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Transport Properties of a Many-Valley Semiconductor

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The simple model of a semiconductor, based on a single effective mass for the charge carriers and a spherical shape for the surfaces of constant energy, is now known to be inadequate for most of the semiconductors which have been extensively studied experimentally. However, some of these do correspond to what may be called the "many-valley" model, a model for which the band edge occurs at a number of equivalent points $\mathbf{K}^{(i)}$ in wave number space, and for which the surfaces of constant energy are multiple ellipsoids, one centered on each of these points. This paper develops, for models of this type, the theory for: mobility (Section 2) and its temperature dependence (Section 3); thermoelectric power (Section 4); piezoresistance (Section 5); Hall effect (Sections 6 and 9); high-frequency dielectric constant (Section 7); and magnetoresistance (Sections 8 and 9). These phenomena are treated, for cases to which Maxwellian statistics apply, on the assumption that the scattering of the charge carriers is describable by a relaxation time which depends on energy only, but is otherwise unrestricted. This assumption can be shown to be justified in a large class of cases, although for some cases it fails, notably when ionized impurity scattering predominates and at the same time the effective mass is very anisotropic. Special attention is given to the role of inter-valley lattice scattering, i.e., to processes whereby a charge carrier is scattered from the neighborhood of one of the band edge points

$\mathbf{K}^{(i)}$ to the neighborhood of a different one. Numerical calculations are presented which show the effects of such processes on the magnitudes and temperature variations of the effects listed above.

1. THE MANY-VALLEY MODEL

Most of the literature of semiconductor theory has been based on what we shall call the simple model. This model is based on the assumption that the minimum energy in the conduction band, or the maximum energy in the valence band, is possessed by only one quantum state of either spin. This state has the form of a Bloch wave with wave number $\mathbf{K} = 0$.* States with energies near the band edge value therefore have small K values, and, since their energies $\epsilon(\mathbf{K})$ must vary continuously with $\mathbf{K}$ in this region, $\epsilon(\mathbf{K})$ for small K must be a quadratic form in K_x, K_y, K_z. If the crystal structure is cubic, $\epsilon(\mathbf{K}) \propto K^2$, and the surfaces of constant energy are spheres in $\mathbf{K}$-space.

It has long been known that other models are possible, and indeed likely in many cases. In recent years it has become clear that the simple model does not apply to *any* of the four cases corresponding to n- and p-type germanium and silicon. The evidence for this includes magnetoresistance[1, 2, 3] and piezoresistance[4] effects, cyclotron resonances,[5] and many other phenomena. Now the possible alternatives to the simple model are the various models for which there is more than one state, apart from spin degeneracy, with the band edge energy. These models fall into two general categories.

(A) Models for which the band edge energy occurs for several wave number vectors $\mathbf{K}^{(i)}$, but for which there is only one state of each spin having this energy and a given $\mathbf{K}^{(i)}$. For a conduction band model of this sort the energy ϵ, considered as a function of $\mathbf{K}$, has a number of minima or "valleys", hence we shall call these "many-valley" or "simple

* For the convenience of the reader the notations defined in the text are recapitulated on page 288.

[1] I. Estermann and A. Foner, Phys. Rev., **79**, p. 365, 1950; G. L. Pearson and H. Suhl, Phys. Rev., **83**, p. 768, 1951; and G. L. Pearson and C. Herring, Physica, to appear.

[2] W. Shockley, Phys. Rev., **78**, p. 173, 1950, and unpublished work.

[3] S. Meiboom and B. Abeles, Phys. Rev., **93**, p. 1121, 1954; B. Abeles and S. Meiboom, Phys. Rev., **95**, p. 31, 1954; and M. Shibuya, J. Phys. Soc., Japan, **9**, p. 134, 1954 and Phys. Rev., **95**, 1385, 1954.

[4] C. S. Smith, Phys. Rev., **94**, p. 42, 1954.

[5] G. Dresselhaus, A. F. Kip, and C. Kittel, Phys. Rev., **92**, p. 827, 1953; B. Lax, H. J. Zeiger, R. N. Dexter, and E. S. Rosenblum, Phys. Rev., **93**, p. 1418, 1954; R. N. Dexter, H. J. Zeiger, and B. Lax, Phys. Rev., **95**, p. 557, 1954; R. N. Dexter, B. Lax, A. F. Kip, and G. Dresselhaus, Phys. Rev., **96**, p. 222, 1954; and R. N. Dexter and B. Lax, Phys. Rev., **96**, p. 223, 1954.

many-valley" models. For a valence band the situation is similar, but inverted.

(B) Models for which, apart from spin degeneracy, there are two or more states with the band edge energy and the same wave number vector. These we shall call "degenerate" models. We may subdivide them further into "degenerate single-valley" and "degenerate many-valley" cases according to whether the band edge energy occurs for only one wave vector, or for several.

This paper is concerned with the transport properties of the simple many-valley models defined under (A). These models are much simpler to handle than the degenerate types, for reasons which are illustrated in Fig. 1. This illustration shows schematically the form in wave number space of the surfaces of constant energy, near the band edge energy, for four models. For the simple model, shown in (a), the locus of a given energy is, as already stated, a sphere. For a simple many-valley model, shown in (b), the locus is a set of ellipsoids centered about the band edge points $\mathbf{K}^{(i)}$. The ellipsoidal shape is required by the facts that energy must depend continuously and differentiably on $\mathbf{K}$ and have an extremum at each $\mathbf{K}^{(i)}$. For a degenerate model, however, the dependence of energy on the components of $\mathbf{K}$ is singular at the band edge point,[2] in that unique second derivatives do not exist: energy varies quadratically with $\mathbf{K}$ in any given direction from this point, but the coefficients going with different directions are determined by a secular equation. The result is that the contours of constant energy may look as shown in Fig. 1(c) (degenerate single-valley case). Degenerate many-valley cases are of course similar, but with the surfaces multiplied, as in Fig. 1(d). Such situations are obviously harder to handle mathematically than those of Fig. 1(b).

Besides the irregularity of the energy surfaces, there is another difference between these two types of cases which greatly complicates theoretical work with degenerate models. This is that in most cases the energies of the two or more states going with a given band-edge $\mathbf{K}$ will be split by spin orbit coupling. If this splitting is $\ll kT$ it can usually be ignored, and if it is $\gg kT$ it may effectively convert the degenerate model into a simple or simple many-valley model. Unfortunately, it usually happens that neither of these extremes applies, and for such intermediate cases not only do we have to deal with energy surfaces like those of Fig. 1(a), but, much worse, the variation of energy with $\mathbf{K}$ is not a simple quadratic dependence even in a fixed direction from the band edge point.

In view of all these complications of the degenerate models, it is for-

tunate that the simple many-valley case does seem to occur for n-type silicon and n-type germanium. One of the hest ways of finding out whether it occurs for any given semiconductor is to compare ohscrvations on this material with theoretical predictions for the various possihle models of the simple many-valley type. We proceed now to derive these predictions, assuming for simplicity that the charge carriers have Maxwellian statistics and an effective relaxation time dependent only on energy. We shall take up the simplest properties first, the more complicated ones later. Sections 2 to 5 will consider perturbation of the distribution function of the carriers hy a static electric field, Section 6

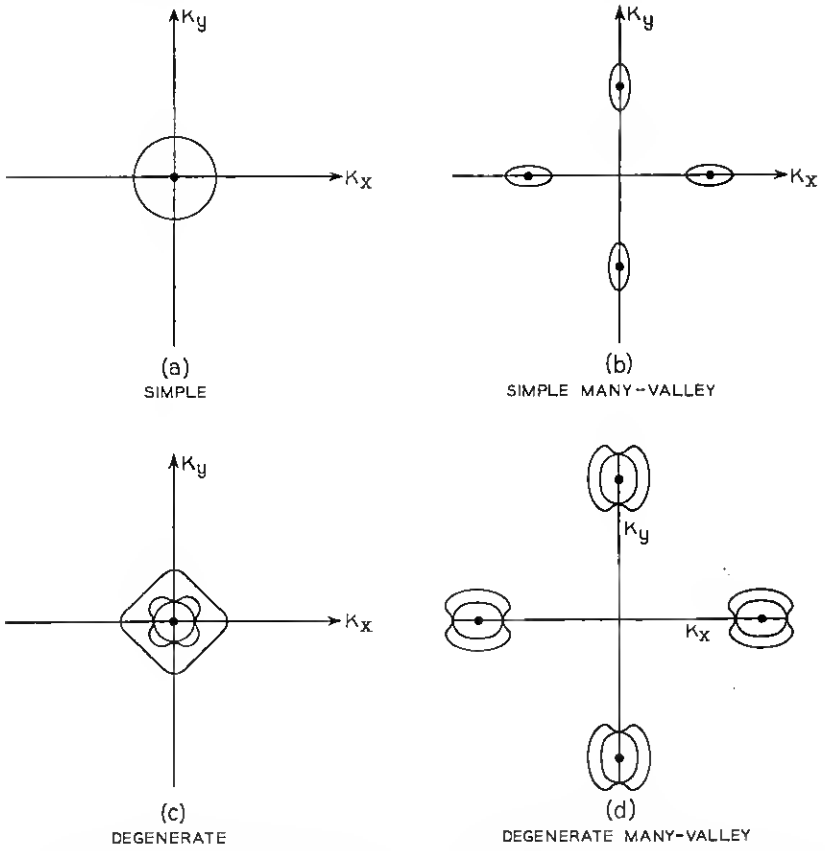

Fig. 1 — Different types of band structure for a semiconductor, illustrated by the forms of the surfaces of constant energy in wave number space. The band edge points are represented by heavy dots.

the Hall effect, Section 7 the perturbation by an oscillating electric field, Section 8 magnetoresistance, and Section 9 effects at high magnetic fields.

In presenting this material our primary objective will be to provide a coherent treatment of all the effects in language as simple and physical as possible. Thus, for example, the Hall and magnetoresistance effects will be discussed *ab initio*, although many of the details presented here have been derived and published independently by several workers.[2, 3] Nor is the theory of this paper the ultimate in refinement: at cost of a little more mathematical complication, the assumption of a relaxation time dependent only on energy can be dispensed with, and anisotropy in the scattering processes acting on the carriers can be taken into account.[6] However, the present simpler treatment illustrates most of the physical principles involved in the various phenomena, and turns out to be quantitatively adequate in a large class of cases.

2. CONDUCTIVITY

In this section we shall solve the Boltzmann equation for the effect of a constant electric field $\mathbf{E}$ on the motion of charge carriers in a simple many-valley band. Maxwellian statistics will be assumed. Thus if $\Delta\mathbf{P} = \hbar(\mathbf{K} - \mathbf{K}^{(i)})$ measures the deviation in crystal momentum space from one of the band edge points $\mathbf{K}^{(i)}$, then for $\mathbf{E} = 0$ the probability of occupation of the state described by $\Delta\mathbf{P}$ (by an electron or hole, depending on the sign of the carriers) is

$$f^{(0)} = \exp\left[\frac{-|\epsilon_F - \epsilon_b| - \frac{\Delta P_1^2}{2m_1^*} - \frac{\Delta P_2^2}{2m_2^*} - \frac{\Delta P_3^2}{2m_3^*}}{kT}\right] \tag{1}$$

where ϵ_F is the Fermi level, ϵ_b the band edge energy and m_1^*, m_2^*, m_3^* are the effective masses in the three coordinate directions 1, 2, 3 which are principal axes for the energy surfaces of the valley in question. When $\mathbf{E} = \neq 0$ the distribution function f is determined by the competition between the perturbing effect of $\mathbf{E}$ and the restoring effect of scattering processes which try to restore the form (1). To make the problem tractable we shall assume that the scattering processes which the charge carriers undergo are described by a relaxation time which is a function of energy ϵ only. In other words, we shall assume that for any slight

[6] C. Herring and E. Vogt, to be published.

departure of f from $f^{(0)}$ the time rate of change of f due to collisions is

$$\left(\frac{df}{dt}\right)_c = -\frac{(f - f^{(0)})}{\tau(\epsilon)} \tag{2}$$

The legitimacy of this assumption is analyzed in Appendix A. It is shown there that the assumption should be rather accurately valid for all kinds of inter-valley scattering — defined as scattering from the neighborhood of one band edge point $\mathbf{K}^{(i)}$ to the neighborhood of another $\mathbf{K}^{(j)}$ — and for intra-valley lattice scattering due to optical modes or to neutral impurities, provided, in tbe latter case, that the temperature is low enough. For intra-valley lattice scattering due to acoustical modes the assumption $\tau = \tau(\epsilon)$ is not necessarily valid, but the arguments of Appendix A suggest tht it will often be a good approximation. For scattering by ionized impurities, however, this assumption will usually be a poor approximation. There is a good prospect that in the near future the adequacy of this approximation for lattice scattering can be quantitatively estimated for some substances. If it should turn out to be inadequate, the necessary generalization of the calculations of this paper can probably be made without great effort.

With the assumptions just stated in (1) and (2), the Boltzmann equation for a steady state in the presence of a field $\mathbf{E}$ takes the form

$$O = \frac{\partial f}{\partial t} = \pm e\mathbf{E}\cdot\nabla_P f - \frac{(f - f^{(0)})}{\tau} \tag{3}$$

where the upper sign is for electrons in a conduction band, the lower for holes in a filled band. If, as is customary, we set

$$f = f^{(0)} + \mathbf{E}\cdot\mathbf{f}^{(1)} + O(E^2), \tag{4}$$

(3) gives, just as in the simple theory,

$$\mathbf{f}^{(1)} = \pm e\tau\nabla_P f^{(0)} \tag{5}$$

Having obtained the solution of the Boltzmann equation in the form (4), (5), we shall now evaluate the electron current density $\mathbf{j}$ from it. If $f^{(0)}$ is Maxwellian,

$$\nabla_P f^{(0)} = \frac{df^{(0)}}{d\Delta\epsilon}\nabla_P\Delta\epsilon = -\frac{\mathbf{v}}{kT} f^{(0)} \tag{6}$$

where $\mathbf{v}$ is the group velocity and $\Delta\epsilon = |\epsilon - \epsilon_b|$ is the distance from the band edge. The contribution of carriers in the ith valley to the current

density is then

$$\mathbf{j}^{(i)} = \sum_{\Delta\mathbf{P}^{(i)},s} (\pm e)\mathbf{v}(\Delta\mathbf{P}^{(i)})f(\Delta\mathbf{P}^{(i)})$$

$$= \frac{e^2}{kT} \sum_{\Delta\mathbf{P}^{(i)},s} f^{(0)}\tau(\Delta\epsilon)\mathbf{E}\cdot\mathbf{vv} \tag{7}$$

where the summations are over all $\Delta\mathbf{P}^{(i)}$ occurring in the ith valley in unit volume of material, and over both states of spin.

The expression (7) states that any single valley i possesses an anisotropic conductivity tensor ${\sigma_{\alpha\beta}}^{(i)}$, or an anisotropic mobility tensor ${\mu_{\alpha\beta}}^{(i)}$, i.e.,

$$j_\alpha{}^{(i)} = \sum_\beta {\sigma_{\alpha\beta}}^{(i)} E_\beta = \sum_\beta (n^{(i)} e{\mu_{\alpha\beta}}^{(i)}) E_\beta \tag{8}$$

where

$$n^{(i)} = \sum_{\Delta\mathbf{P}^{(i)},s} f^{(0)} \tag{9}$$

is the number of carriers in valley i per unit volume. If we choose the x, y, and z axes to be along the principal axes of the ellipsoidal energy surfaces of valley i, (7) shows that ${\sigma_{\alpha\beta}}^{(i)}$ and ${\mu_{\alpha\beta}}^{(i)}$ will be diagonal. Each diagonal element ${\mu_{\lambda\lambda}}^{(i)}$ will involve a Maxwellian average of ${v_\lambda}^2\tau(\Delta\epsilon)$. Now the equipartition principle leads us to expect that the average, over an energy shell $\Delta\epsilon$ to $\Delta\epsilon + d\Delta\epsilon$ in $\Delta\mathbf{P}$-space, of the kinetic energy associated with the x-component of velocity should be the same as that associated with the y- or z-component. This is easily demonstrated explicitly (Appendix B). Thus, if $m_1{}^*$, $m_2{}^*$, $m_3{}^*$ are the effective masses in the three principal directions,

$$\tfrac{1}{2}\, m_1{}^* {v_1}^2 = \tfrac{1}{2}\, m_2{}^* {v_2}^2 = \tfrac{1}{2}\, m_3{}^* {v_3}^2 \tag{10}$$

Therefore (7) and (8) give, in our system of axes,

$${\mu_{\alpha\alpha}}^{(i)} = \frac{e}{m_\alpha{}^*} \frac{\langle\Delta\epsilon\tau\rangle}{\langle\Delta\epsilon\rangle} \tag{11}$$

$${\mu_{\alpha\beta}}^{(i)} = 0 \qquad (\alpha \neq \beta) \tag{12}$$

where the angular brackets denote Maxwellian averages:

$$\langle\Delta\epsilon\tau\rangle = \sum_{\Delta\mathbf{P}} \Delta\epsilon\tau f^{(0)} / \sum_{\Delta\mathbf{P}} f^{(0)}, \text{ etc.} \tag{13}$$

The denominator of (11), $\langle\Delta\epsilon\rangle$, of course equals $\frac{3}{2}\, kT$ by equipartition.

The formula (11), it will be noted, is the same as that of the simple theory[7] with m^* replaced by $m_\alpha{}^*$.

The overall conductivity tensor due to the carriers in all the valleys is of course $\sum_i \sigma_{\alpha\beta}{}^{(i)}$, and the overall mobility tensor is the average of $\mu_{\alpha\beta}{}^{(i)}$ over the different valleys. For a cubic crystal the mobility is the same in all directions, so we have

$$\begin{aligned} \mu &= \mu_{\lambda\lambda} = \tfrac{1}{3} \sum_\alpha \mu_{\alpha\alpha} = \frac{1}{3N_V} \sum_i \sum_\alpha \mu_{\alpha\alpha}{}^{(i)} \\ &= \frac{e}{m^{(I)}} \frac{\langle \Delta\epsilon\tau \rangle}{\langle \Delta\epsilon \rangle} \end{aligned} \tag{14}$$

where N_V is the number of valleys and $m^{(I)}$ is an average inertial mass defined by

$$\frac{1}{m^{(I)}} = \tfrac{1}{3} \left[\frac{1}{m_1{}^*} + \frac{1}{m_2{}^*} + \frac{1}{m_3{}^*} \right] \tag{15}$$

This mass, as we shall see in Section 7, is the one most directly measured by the Benedict-Shockley experiment on high-frequency dielectric constant.

3. TEMPERATURE VARIATION OF LATTICE MOBILITY

The τ occurring in the mobility expression (14) differs from the τ of the simple model in that it contains the effect of inter-valley scattering in addition to intra-valley and impurity scattering. Inter- and intra-valley scattering differ in that most of the phonons emitted or absorbed in intra-valley scattering have energies $\ll$ the energies of the charge carriers, while those involved in inter-valley scattering usually do not. If $\mathbf{K}^{(i)}$ and $\mathbf{K}^{(j)}$ are two different band edge points, scattering of a carrier from valley i to valley j must involve emission or absorption of a phonon of wave number close to $\pm\mathbf{q}_{ij}$, where $\mathbf{q}_{ij} = \mathbf{K}^{(i)} - \mathbf{K}^{(j)}$. If $\mathbf{q}_{ij}$ has a magnitude of the order of the radius of the Brillouin zone, as is likely in most cases, the energy $\hbar\omega_{ij}$ of this phonon will be a major fraction of of $k\Theta$, where Θ is the Debye temperature. This is usually $\geqq kT$ in the extrinsic range. One must therefore use the Planck, rather than the Rayleigh-Jeans, distribution function for these phonons. At very low temperatures, inter-valley scattering is negligible: absorption of an ij phonon is rare because few such phonons are present; emission is com-

[7] See, for example, W. Shockley, *Electrons and Holes in Semiconductors*, (Van Nostrand 1951) p. 276.

parahly rare hecause few carriers have energy enough to create such a phonon. With rising temperature inter-valley scattering becomes more important. This causes τ (hence μ) to decrease more rapidly with increasing T than it would if there were no inter-valley scattering. In this section we shall develop this idea quantitatively.

The matrix element for scattering of a carrier from some state in valley i to another state in valley j, hy ahsorption or emission of a phonon $\hbar\omega$, has the form common to all one-phonon scattering processes[8]

$$M_{ij} = \left.\begin{matrix} N^{1/2} \\ (N+1)^{1/2} \end{matrix}\right\} D_{ij} \text{ for } \begin{cases} \text{ahsorption} \\ \text{emission} \end{cases} \tag{16}$$

where N is the numher of phonons of the given type present in the initial state and whcre D_{ij} is independent of the occupation of the phonon states. For inter-valley scattering D_{ij} is practically independent of the locations of the initial and final states in their respective valleys. In general, of course, D_{ij} will be different for the different hranches of the vihrational spectrum. The transition probability from a statc of energy ϵ in valley i to a state in valley j of energy $\epsilon' = \epsilon + \hbar\omega$ (ahsorption) or $\epsilon - \hbar\omega$ (emission) is proportional to $|M_{ij}|^2$ times the dcnsity of states at energy ϵ' in the jth valley, provided thc variation of $\hbar\omega$ with position in the valley is negligible, as is the case for most transitions. Since the numher of states hetween ϵ' and $\epsilon' + d\epsilon'$ is proportional to $\Delta\epsilon'^{1/2}\, d\Delta\epsilon'$, where $\Delta\epsilon'$ is the distance from the band edge, this transition probability has the form

$$\text{ahsorption: } W_a \propto \frac{(\epsilon + \hbar\omega)^{1/2}}{\exp(\hbar\omega/kT) - 1} \tag{17}$$

$$\text{emission: } W_e \propto \begin{cases} \dfrac{(\Delta\epsilon - \hbar\omega)^{1/2}}{1 - \exp(-\hbar\omega/kT)} & \text{for } \Delta\epsilon > \hbar\omega \\ 0 & \text{for } \Delta\epsilon < \hbar\omega \end{cases} \tag{18}$$

Since either of the processes (17) and (18) randomizes the initial velocity of the charge carriers, and since in this paper we are assuming the existence of an effectivc relaxation time $\tau_{ii}(\epsilon)$ for randomization of velocity by the intra-valley scattering of acoustic modes, the total relaxation time for lattice scattering is given hy

$$\frac{1}{\tau} = \frac{1}{\tau_{ii}} + \sum_{j,\alpha}{}' [W_a(ij,\alpha) + W_e(ij,\alpha)] \tag{19}$$

where α lahels the hranches of the vihrational spectrum and W_a and W_e

[8] See, for example, Reference 7, p. 520.

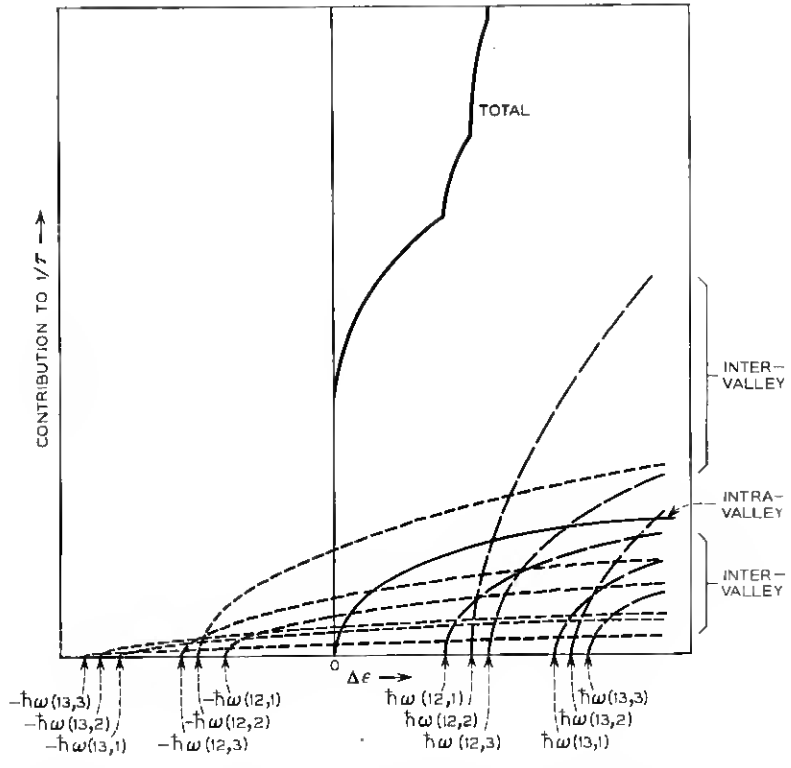

Fig. 2 — Contributions to the reciprocal relaxation time of a charge carrier, due to inter-valley and intra-valley lattice scattering. The dot-dash curves are the inter-valley scattering contributions $W_e(ij, \alpha)$ for emission of a phonon, the dashed curves are the corresponding quantities $W_a(ij, \alpha)$ for absorption of a phonon. There are many transitions from valley 1 to different ones of the other valleys, due to different branches α of the phonon spectrum.

are given for each type of transition by (17) and (18) respectively, with $\hbar\omega = \hbar\omega(ij, \alpha)$. The prime on the summation means that when α is an acoustic branch, the term $j = i$ is to be omitted. However, since (17) and (18) apply to intra-valley scattering by modes of the optical branches, such scattering is included in (19) as the terms with $j = i$. Fig. 2(a) shows the various contributions to $1/\tau$ as functions of the initial energy $\Delta\epsilon$ of the carrier being scattered: $1/\tau_{ii}$ is proportional to $\Delta\epsilon^{1/2}$, as in the simple theory (this corresponds to a mean free path independent of energy for any given direction of motion), and each of the other terms is proportional to some $(\Delta\epsilon \pm \hbar\omega)^{1/2}$.

We shall try to estimate the order of magnitude of the steepness of

the parabolas describing the various inter-valley terms, relative to that of the intra-valley term $1/\tau_{ii}$. For the low-frequency acoustic modes involved in intra-valley scattering the factor D_{ij} in the matrix element (16) is proportional to $q/(\hbar\omega)^{1/2}$, and since $\omega \propto q$ and $N \approx kT/\hbar\omega \gg 1$ for such modes $|M_{ij}|^2 \propto T$ and is independent of q. The q's involved in inter-valley scattering will usually be too large to satisfy $kT/\hbar\omega \gg 1$, at least in the extrinsic ranges of Ge and Si, but we may hope to estimate a plausible order of magnitude for their W_a's and W_e's by assuming their D_{ij}'s to be $\propto q/\hbar\omega$ with a factor of proportionality of the same order as for intra-valley scattering. With this assumption the steepness of a typical (ij) parabola corresponding to phonon emission (W_e) should be of the same order as the steepness of the intra-valley parabola when $kT \geqq \hbar\omega(ij)$, while for $kT < \hbar\omega(ij)$ the $W_e(ij)$ parabola should become nearly independent of T, as contrasted with $1/\tau_{ii}(\epsilon) \propto T$. The parabolas corresponding to phonon absorption are of course always less steep, the ratio of the steepness of $W_a(ij)$ to that of $W_e(ij)$ being

$$\frac{W_a/(\Delta\epsilon + \hbar\omega)^{1/2}}{W_e/(\Delta\epsilon - \hbar\omega)^{1/2}} = \frac{1 - \exp(-\hbar\omega/kT)}{\exp(\hbar\omega/kT) - 1} = \exp(-\hbar\omega/kT) \qquad (20)$$

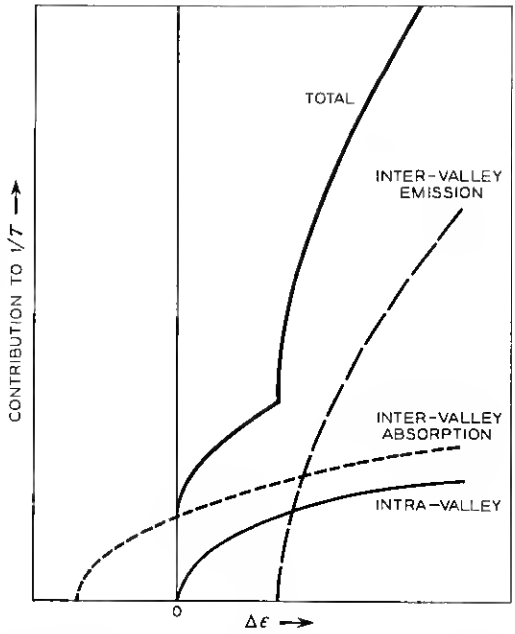

Fig. 3 — Same as Fig. 2, but for the simplified model of Equation (24), on which the numerical calculations of Figs. 4, 5, 8, 9 and 10 are based.

Because of the large number of terms $W_{a,e}(ij, \alpha)$ in (19) or Fig. 2, each with an at present unknown amplitude and critical frequency, it would be pointless to undertake calculations taking individual account of all the possible types of transitions. However, it is reasonable to hope that the behavior of the inter-valley terms can be roughly approximated by a model which considers absorption and emission of just a single type of inter-valley phonon. This model is illustrated in Fig. 3. It contains three adjustable parameters w_1, w_2, and $\hbar\omega$, defined by

$$1/\tau_{ii} = w_1 \left(\frac{\Delta\epsilon}{\hbar\omega}\right)^{1/2} \left(\frac{kT}{\hbar\omega}\right) \tag{21}$$

$$W_a = \frac{w_2 \left(\frac{\Delta\epsilon}{\hbar\omega} + 1\right)^{1/2}}{\exp\,(\hbar\omega/kT) - 1} \tag{22}$$

$$W_e = \frac{w_2 \left(\frac{\Delta\epsilon}{\hbar\omega} - 1\right)^{1/2}}{1 - \exp\,(-\hbar\omega/kT)} \text{ or } 0 \tag{23}$$

Equation (19) becomes

$$w_1\tau = \left\{\left(\frac{\Delta\epsilon}{\hbar\omega}\right)^{1/2}\left(\frac{kT}{\hbar\omega}\right) + \frac{w_2}{w_1}\left[\frac{\left(\frac{\Delta\epsilon}{\hbar\omega} + 1\right)^{1/2}}{\exp\,(\hbar\omega/kT) - 1} + \frac{\left(\frac{\Delta\epsilon}{\hbar\omega} - 1\right)^{1/2} \text{ or } 0}{1 - \exp\,(-\hbar\omega/kT)}\right]\right\}^{-1} \tag{24}$$

Thus $w_1\tau$ is a function of the two variables $\Delta\epsilon/\hbar\omega$ and $kT/\hbar\omega$, and the single parameter w_2/w_1. The behavior of the mobility as a function if $kT/\hbar\omega$ therefore depends, apart from the constant scale factor w_1, only on w_2/w_1.

Fig. 4 shows the results of some calculations of this mobility-temperature relation, made by numerical evaluation of (24) and (14). It is evident that with reasonable values of w_2/w_1, the negative exponent describing the temperature variation of the mobility can be increased to a value considerably above the $\frac{3}{2}$ of the simple theory, over a considerable range of temperature. This is often what is needed to explain the observed mobility behavior. In Sections 4, 6, and 8 we shall see the extent to which this mobility exponent is correlated with, respectively, the electronic part of the thermoelectric power, the ratio of Hall to drift mobility, and the magnitude of the magnetoresistance.

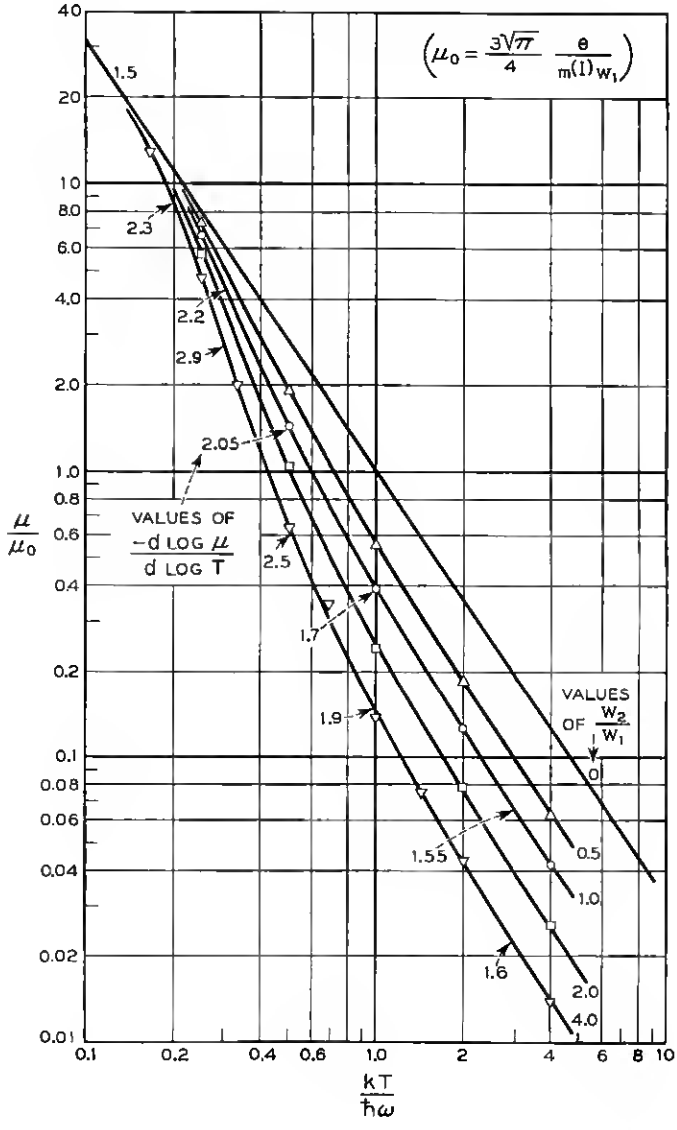

Fig. 4 — Mobility-temperature curves for pure lattice scattering, as obtained from the simplified expression (24) for the relaxation time. The quantities w_1 and w_2 measure the strength of the coupling of the carriers to intra- and inter-valley modes, respectively; ω is the frequency of the inter-valley mode. The curves have been drawn so as to smooth out irregularities in the computed points.

4. THERMOELECTRIC POWER

The thermoelectric power of a semiconductor is a little different from the other effects discussed in this paper, in that it involves not only the response of the distribution function of the charge carriers to a perturbing temperature gradient or electric field, but also the alteration of the distribution function of the phonon system.[9, 10] The duality manifests itself in the apperaance of two contributions to the thermoelectric power Q: the measured Q is the sum of an electronic part Q_e, representing the emf necessary to counteract the tendency of charge carriers to diffuse from hot regions to cold, and a phonon part Q_p, representing the emf necessary to counteract the drag exerted on the carriers by the phonons which flow down the temperature gradient in thermal conduction. As the present paper is devoted to effects having to do with the response of the electronic distribution function to various influences, and as all aspects of the theory of thermoelectric power have been discussed elsewhere,[10] we shall limit the present section to a discussion only of the electronic part Q_e, which, fortunately, predominates greatly over Q_p at high temperatures.

The expression for Q_e is most simply derived by making use of the Kelvin relation $Q_e = \Pi_e/T$ between Q_e and the electronic contribution Π_e to the Peltier coefficient, which represents the energy flux, relative to the Fermi level, which accompanies the transport of unit charge in an isothermal conduction process. For an intrinsic semiconductor with low carrier concentration

$$eTQ_e = e\Pi_e = \epsilon_F - \epsilon_b - \Delta\epsilon_T \tag{25}$$

where as before ϵ_F is the Fermi level, ϵ_b the band edge energy, and where $\Delta\epsilon_T$ is the average energy of the transported electrons relative to the band edge, a quantity >0 for n-type material, <0 for p-type, and of the order of magnitude of kT. Now $|\epsilon_F - \epsilon_b|$ can be expressed in terms of the carrier concentration n and the effective masses. For a many-valley model the number of carriers $n^{(i)}$ in each valley is easily shown to be the same as for a simple model semiconductor with the same $|\epsilon_F - \epsilon_b|$ and with an effective mass equal to the geometric mean of the principal masses m_1^*, m_2^*, m_3^* of the valley. This is because the density of states in energy is proportional to the volume of K-space inside an energy surface, a quantity which for a spherical surface goes as the cube of the radius, and for an ellipsoidal one as the product of the principal semi-

[9] H. P. R. Frederikse, Phys. Rev., **92**, p. 248, 1953.
[10] C. Herring, Phys. Rev., **96**, p. 1163, 1954.

axes. The total carrier concentration is therefore

$$n = N_V n^{(i)} = \frac{2(2\pi kT)^{3/2}}{h^3} (m_1^* m_2^* m_3^*)^{1/2} N_V \exp\left(-\frac{|\epsilon_F - \epsilon_b|}{kT}\right)$$

where N_V is the number of valleys. The final expression for Q_e obtained by expressing $|\epsilon_F - \epsilon_b|$ in terms of n and inserting in (25) is

$$Q_e = \mp 86.2 \left[\ln \frac{4.70 \times 10^{15}}{n} + \tfrac{3}{2} \ln N_V + \tfrac{1}{2} \ln \left(\frac{m_1^*}{m} \cdot \frac{m_2^*}{m} \cdot \frac{m_3^*}{m} \right) + \tfrac{3}{2} \ln T + \frac{|\Delta\epsilon_T|}{kT} \right] \mu v/\text{deg}. \tag{26}$$

where n is in cm^{-3} and the upper sign is for n-type material, the lower for p-type.

If a relaxation time exists, dependent only on energy, the distribution function for isothermal conduction has the form $f^{(0)} + \mathbf{E} \cdot \mathbf{f}^{(1)}$ worked out in Section 2, and we have, for a cubic crystal,

$$|\Delta\epsilon_T| = \frac{\int \Delta\epsilon \mathbf{v} \cdot \mathbf{f}^{(1)} \, d\mathbf{P}}{\int \mathbf{v} \cdot \mathbf{f}^{(1)} \, d\mathbf{P}} = \frac{\langle \Delta\epsilon^2 \tau \rangle}{\langle \Delta\epsilon \tau \rangle} \tag{27}$$

by (5), (6) and (10), where as before the angular brackets denote Maxwellian averages as defined by (13).

It is important to know the value of (27) as accurately as possible, in the temperature range where Q_e is measurable, since if (27) is known the measured Q_e can be used with (26) to give information on the effective masses. For pure intra-valley scattering, (27) has the value $2kT$. Impurity scattering increases $\Delta\epsilon_T$ by causing the current to be carried more by fast carriers and less by slow; inter-valley scattering has the reverse effect. It is worth while to try to correlate the effect of inter-valley scattering on $\Delta\epsilon_T$ with its effects on two measurable properties, namely, the temperature variation of mobility (Section 3) and the ratio of Hall to drift mobility (Section 6). Accordingly, calculations of $|\Delta\epsilon_T|$ have been made using the expression (24) (model of Fig. 3) for the relaxation time. The results are shown in Fig. 5, which shows $|\Delta\epsilon_T|/kT$ as a function of $kT/\hbar\omega$.

5. PIEZORESISTANCE

As we have just seen in Section 2, the quantum states in any small region of wave number space make a contribution to the conductivity

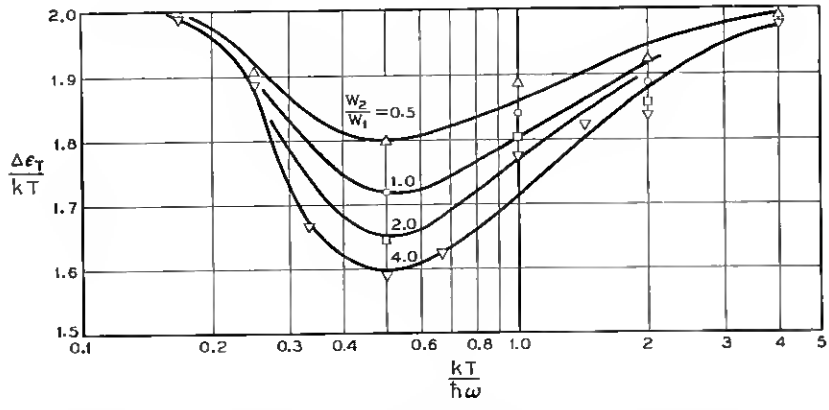

Fig. 5 — Values of the thermoelectric transport ratio $|\Delta\epsilon_T|/kT$ defined by (27), for the simplified lattice scattering law (24). The ratio w_2/w_1 measures the strength of the coupling of the carriers to inter-valley modes in terms of that for intra-valley scattering; ω is the frequency of the inter-valley modes. The curves have been drawn to smooth out irregularities (severe for $kT/\hbar\omega$ = 1 to 2) in the calculated points.

which depends on (i) *the degree to which these states are populated* in the equilibrium distribution $f^{(0)}$, (ii) *their group velocity*, and (iii) *their relaxation time*, or more generally, the transition probabilities for scattering from these states to others. When the crystal is strained, any or all of these factors may change, and the resulting change in the sum of all the local contributions to the conductivity constitutes the piezoresistance effect recently discovered by Smith.[4] Although there are a number of processes which can contribute to the three factors (i) to (iii) just enumerated, it can be argued plausibly that for a simple many-valley model the principal effects are usually those due to a single process, namely, the strain-induced shifts of the energies ϵ_i of the band edge points $\mathbf{K}^{(i)}$. We shall consider (i) to (iii) in turn:

(i) The change in the population $f^{(0)}(\mathbf{K}^{(i)} + \Delta\mathbf{K})$ depends on the shift of the energy $\epsilon(K^{(i)} + \Delta\mathbf{K})$, and because of the smallness of $\Delta\mathbf{K}$ this is practically the same as the shift $\delta\epsilon^{(i)}$ of $\epsilon(\mathbf{K}^{(i)})$. In a shearing strain some of the $\delta\epsilon^{(i)}$ will be positive, some negative, and so some of the valleys will have their populations decreased, some increased, the fractional change in each case being $\delta\epsilon^{(i)}/kT$. Now it is evident from the second equation of (7) that the contribution of a single valley to the conductivity is anisotropic. If all valleys are populated equally, as we assumed in Section 1, the total conductivity will be isotropic. But if strain causes different valleys to have different populations, the overall conductivity will have

an anisotropy like that of the more populous valleys. If the ratio of $\delta\epsilon^{(i)}$ to the shear strain amplitude is of the order of magnitude of the known ratio of $\delta\epsilon_G$ to strain for isotropic compression, viz., a few volts, the fractional change of $f^{(0)}$ per unit strain will be of the order of hundreds. Since the observed fractional change in resistance per unit shear strain is of the order of 10^2 in the more favorable orientations,[4] the change in $f^{(0)}$ is of the right order of magnitude to contribute a major part of the effect.

For an isotropic compression or dilation there exists the possibility, not present for shearing strains, that the total carrier concentration may be changed in first order. A large effect of this sort, again of the order of the $\delta\epsilon^{(i)}/kT$, will occur for a specimen in or near the intrinsic range, because of the change of energy gap ϵ_G with strain. This effect rapidly becomes negligible, however, as the specimen is made extrinsic. For example, if unit volume of an n-type specimen has an excess n_D of donors over acceptors, all ionized, the hole and electron concentrations n_h, n_e, obey

$$n_e = n_D + n_h, \qquad n_e n_h = n_i^2$$

where $n_i(T)$ is the value of $n_e = n_h$ in intrinsic material. Thus if $n_D \gg n_i$

$$\frac{n_h}{n_D} = \left(\frac{n_i}{n_D}\right)^2 \tag{28}$$

and since $\partial n_e/\partial\epsilon_G = \partial n_h/\partial\epsilon_G$, the energy gap effect is negligible if n_D exceeds n_i by a large factor, even though the change in n_i with strain may be sizable. For extrinsic specimens with incomplete ionization of impurity centers, there may of course be an effect of compression on total carrier concentration due to change in the ionization energy of the centers; however, if this ionization energy is $\ll\epsilon_G$ this effect will be of a smaller order of magnitude than the $\delta\epsilon^{(i)}/kT$.

(ii) It is easy to show that the fractional change in group velocity per unit strain must be much smaller than the $\delta\epsilon^{(i)}/kT$ just discussed, hence too small to contribute in a major way to the piezoresistance effect. For we expect the change $\delta\mathbf{v}$ in the group velocity at $\mathbf{K}^{(i)} + \Delta\mathbf{K}$ to have an order of magnitude given by

$$\delta v \sim [\delta\epsilon(\mathbf{K}^{(i)} + \Delta\mathbf{K}) - \delta\epsilon^{(i)}]/\hbar\Delta K \sim (\Delta K/K^{(i)})^2(\delta\epsilon^{(i)}/\hbar\Delta K)$$

since the quantity in square brackets must vary as ΔK^2. Since

$$v \sim [\epsilon(\mathbf{K}^{(i)} + \Delta\mathbf{K}) - \epsilon^{(i)}]/\hbar\Delta K = \Delta\epsilon/\hbar\Delta K$$

we have

$$\delta v/v \sim (\Delta K/K^{(i)})^2(\delta\epsilon^{(i)}/\Delta\epsilon) \tag{29}$$

Since a typical charge carrier has $\Delta\epsilon \sim kT$, (29) is smaller than the ratio discussed in the preceding paragraph by the factor $(\Delta K/K^{(i)})^2$. It is thus plausible to neglect strain-induced changes in group velocity, or equivalently, in the effective masses.

(iii) Consider the transition probability from a state $\mathbf{K}$ to the group of states lying in a small element of volume in $\mathbf{K}$-space, centered on a point $\mathbf{K}'$ at which the proper energy conservation law for the transition $\mathbf{K} \rightarrow \mathbf{K}'$ is satisfied. This probability, like all quantum-mechanical transition probabilities, can be expressed as the product of the square of a matrix element $M(\mathbf{K}, \mathbf{K}')$ by the number of states per unit energy in the given element of volume. We have to consider the effect of strain on each of these factors.

The matrix element $M(\mathbf{K}, \mathbf{K}')$ can be changed either by a change in the wave functions Ψ_K, $\Psi_{K'}$, or by a change in the physical processes determining the perturbation operator M, e.g., a change in the amplitudes of the thermal vibrations, or a change in the dielectric constant, which enters into scattering by charged impurities. Typical assumptions on the equation of state of a crystal suggest that the fractional change in the squared vibration amplitude, per unit strain, might be of the order of a few units, i.e., at least an order of magnitude less than the observed elastoresistance for the optimum orientations. The effect of the change in the wave functions is of similar magnitude: To effect a major change in $M(\mathbf{K}, \mathbf{K}')$ one must make a major change in the wave functions. To do this probably usually requires a strain of amplitude 0.1 to 1. Therefore it is reasonable to expect that the fractional change in $|M^2|$ per unit strain will be of the order of 10 or less, i.e., again an order of magnitude smaller than $\delta\epsilon^{(i)}/kT$, or than the observed elastoresistance.

The effect of strain on the density-of-states factor, on the other hand, can be larger. For intra-valley scattering, where initial and final states are both near the same band edge point $\mathbf{K}^{(i)}$, the effect is of course very small, since initial and final states undergo very nearly the same energy shift with strain. But for scattering from one valley i to another valley j, the two energy shifts $\delta\epsilon^{(i)}$ and $\delta\epsilon^{(j)}$ are in general quite different, and for a given initial state application of a strain will change the set of $\mathbf{K}'$s describing final states which conserve energy and hence will change the density of final states — e.g., the density in a given solid angle of vectors $\Delta\mathbf{K}' \equiv \mathbf{K}' - \mathbf{K}^{(j)}$. Since in a given solid angle the density of states is $\propto \Delta\epsilon'^{1/2}$, the fractional change in this density due to a strain is $\delta\epsilon^{(j)}/2\Delta\epsilon'$, which on the average is of the order of $\delta\epsilon^{(j)}/kT$, i.e., of the same order as the effect discussed under (i).

TABLE I — WAYS IN WHICH STRAIN CAN AFFECT CONDUCTIVITY

Effect	Probable Order of Magnitude	Rank in Importance
(i) Population function $f^{(0)}$	$\delta\epsilon^{(i)}/kT$ + much smaller terms	First
(ii) Group velocities of states	$\ll\delta\epsilon^{(i)}/kT$	
(iii) Transition probabilities		
(a) Matrix elements		
(α) Wave functions	$\ll\delta\epsilon^{(i)}/kT$	
(β) Vibration amplitudes, etc.	Rather $<\delta\epsilon^{(i)}/kT$	Second (?)
(b) Density of states		
(α) Intravalley	$\ll\delta\epsilon^{(i)}/kT$	
(β) Intervalley	$\delta\epsilon^{(i)}/kT$ + much smaller terms	First

Table I summarizes the foregoing discussion of the ways in which strain can affect conductivity.

Appendix C gives the mathematical treatment of the two effects which are of the order of the quantities $\delta\epsilon^{(i)}/kT$, namely, the change in $f^{(0)}$ and the change in the density-of-states factor in the transition probabilities for inter-valley scattering. This treatment, which is fairly simple and straightforward, is based on the following assumptions:

(a) Neglect of all other effects of strain on the conductivity.

(b) The assumption of the preceding sections that the scattering of the carriers is describable by a relaxation time which in each valley is a function of energy only.

(c) Carrier concentrations in the extrinsic range.

(d) Maxwell-Boltzmann statistics.

(e) Valleys lying along a threefold or fourfold symmetry axis of a cubic crystal. For such valleys the energy surfaces are ellipsoids of revolution.

The principal features of the calculation are qualtative ones which can be derived with little or no mathematics. These we shall consider here, with a little inquiry in each case as to the sensitivity of the conclusion to relaxation of the assumptions (a) and (e) above. The first such feature to be noted is that *under assumption (a) the change of mobility in an isotropic compression vanishes.* For in an isotropic compression all the band edge shifts $\delta\epsilon^{(i)}$ are equal. This means that for a given total carrier density the distribution function $f^{(0)}$ in each valley does not change, if, as we are doing, we neglect changes in the effective masses. Similarly, since all valleys are shifted together, there is no change in the density of final states corresponding to any inter-valley scattering process. The present conclusion is easily seen to be independent of

TABLE II — ISOTHERMAL ELASTORESISTANCE CONSTANTS FOR Ge AND Si (SMITH, REFERENCE 4)

Material and Resistivity		$m_{1212} \equiv m_{44}$	$\frac{m_{1111} - m_{1122}}{2} \equiv \frac{m_{11} - m_{12}}{2}$	$-\frac{1}{\sigma}\frac{d\sigma}{d\,\ln V} = \frac{m_{11} + 2m_{12}}{3}$
	Ω cm			
n Ge	1.5	−93.0	+0.4	−5.3
	5.7	−92.0	+0.5	−6.8
	9.9	−92.8	+0.1	−9.8
	16.6	−93.4	+0.1	−13.6
p Ge	1.1	+65.1	−2.8	+3.9
	15.0	+66.5	−6.3	+1.4
n Si	11.7	−10.8	−79.5	+5.7
p Si	7.8	+110.0	+3.9	+6.0

Here $m_{\rho\nu\sigma\beta}$, defined by (C7) of Appendix C, describes the relative change of the conductivity tensor with the strain tensor, in a coordinate system oriented along the cube axes. The abbreviation of this by $m_{rs}(r, s = 1 \text{ to } 6)$ follows the same practice as that used for elastic constants.

assumptions (b), (d), and (e). As regards assumption (a), however, it is clear that inclusion of any of the other strain effects listed in Table I will in general lead to a nonvanishing effect of compression on the mobility.

By virtue of the fact just mentioned it is possible to test the validity of assumption (a) by comparing the observed elastoresistance for isotropic compression with that for a typical shear. Table II, taken from the work of Smith,[4] shows the room temperature elastoresistance constants of Ge and Si. The entries in the last column vary with resistivity for the case of Ge, because of the energy gap effect discussed under (i) above [failure of assumption (c)]; our present interest is therefore in the values for low resistivity specimens. For these the volume coefficient (last column) is in all cases only a few percent of the larger of the shear coefficients (middle columns); this accords with the expectation that the volume variation of the squared matrix element for scattering (presumably the largest of the neglected effects) should be an order of magnitude or more smaller than the $\delta\epsilon^{(i)}/kT$. This is encouraging, but it must be remembered that the shear variation of the matrix element may well be larger than its volume variation because suitable shearing strains can usually couple a band edge state to states closer to it in energy than can isotropic dilatation.

The second important conclusion is that *under assumption (a) the change of mobility vanishes for a dilatation along a (100) direction if the valleys are on (111) axes, and for a dilatation along a (111) direction, if the valleys are on (100) axes.* In terms of the elastoresistance coefficients of Table II, $(m_{11} - m_{12})$ vanishes for (111) valleys, and m_{44} vanishes for (100) valleys. This conclusion is obvious from the symmetry of the

problem: a shear compounded out of a unidirectional dilatation of the type described and an isotropic compression must shift all band edge points by the same amount. This amount must be the same as in the negative of this shear, so all $\delta\epsilon_i = 0$. This conclusion is again independent of assumptions (b) and (d), but in general breaks down if assumption (a) is relaxed to the extent of taking account of the effect of strain on the matrix element for scattering.

The third point to be made is that *the change of mobility accompanying a given strain is inversely proportional to T at temperatures low enough for inter-valley scattering to be of negligible importance.* This is because the relative change of population of different valleys with strain is proportional to the $\delta\epsilon^{(i)}/kT$. The more complete treatment of Appendix C shows that, under the present assumptions, the decrease of elastoresistance with increasing T should be more rapid than $1/T$ when inter-valley scattering is just becoming important, but that for very high T it should again go as $1/T$. This behavior is illustrated schematically in Fig. 6. The present conclusion is not dependent on assumptions (b) or (e), but depends on the others, especially (a). The effect of strain on the matrix elements for scattering will give a contribution to the elastoresistance which is independent of T in the range (if such exists) where only intra-valley lattice scattering is important; if impurity or inter-valley scattering contributes the dependence is of course more complicated.

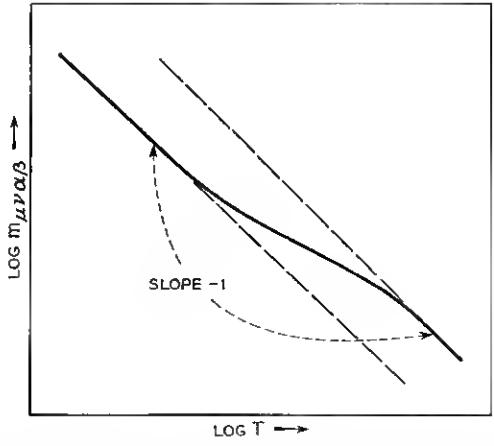

Fig. 6 — Schematic variation of any component of elastoresistance with temperature, showing the transition from the low temperature region where the only important effect of strain is to change the relative population of the valleys, to the high temperature region where the effect of strain on inter-valley scattering is of comparable importance.

In conclusion, a few words are in order regarding the extent to which the present conclusions on piezoresistance can be expected to hold for models other than the simple many-valley type to which this memorandum is restricted. First of all, we may note that for the various types of degenerate models, such as that of Fig. 1(a), different states in the neighborhood of the same band edge point can experience widely different energy shifts $\delta\epsilon$ under shear. Consequently the mobility will be affected in a major way not only by the two effects labeled "first" in Table I — change of the population function and change of the density-of-states function in inter-valley scattering — but also by changes in the group velocities. Moreover, the perturbation of the crystal Hamiltonian by a uniform shearing strain may now have sizable matrix elements between states of the same wave vector belonging to the different bands which come together at the band edge point. This can cause the form of the crystal wave functions to be much more sensitive to strain than when the perturbation only connects states a few volts apart in energy, and so the dependence on strain of the matrix element for scattering may be much larger than for the simple many-valley case. Thus at least four, rather than two, of the entries in Table I become of first magnitude.

In view of these facts, most of the conclusions reached for the simple many-valley case probably become invalid for the degenerate and degenerate many-valley cases. An exception is the conclusion concerning the smallness of the change of mobility in isotropic compression. The perturbation introduced into the crystal Hamiltonian by an isotropic compression does not mix states of a degenerate set, so the arguments previously given remain valid.

6. HALL EFFECT AT LOW H

When a magnetic field is present the $\mathbf{E}$ in the transport equation (3) must be replaced by $\mathbf{E} + \mathbf{v} \times \mathbf{H}/c$, where as before, $\mathbf{v}$ is the group velocity. Thus with the upper sign for electrons, the lower for holes, the distribution function f of the carriers obeys

$$0 = \frac{\partial f}{\partial t} = \pm \left[e\mathbf{E} \cdot \nabla_p f + e \frac{\mathbf{v} \times \mathbf{H}}{c} \cdot \nabla_p f \right] - \frac{(f - f^{(0)})}{\tau} \tag{30}$$

We shall seek the solution of this as far as the first order in $\mathbf{E}$ and the first order in $\mathbf{H}$, i.e., we shall set

$$f = f^{(0)} + \mathbf{E} \cdot \mathbf{f}^{(10)} + \sum_{\mu\nu} E_\mu H_\nu f_{\mu\nu}^{(11)} + \cdots \tag{31}$$

There is, of course, no term of the first order in $\mathbf{H}$ and the zeroth in $\mathbf{E}$,

since a pure magnetic field has no effect on f. The vector function $\mathbf{f}^{(10)}$ is of course the same as in Section 2, Equation (5), namely,

$$\mathbf{f}^{(10)} = \pm e\tau \nabla_P f^{(0)} \tag{32}$$

Putting (32) and (31) into (30) we get for $f_{\mu\nu}{}^{(11)}$:

$$\frac{1}{\tau} \sum_{\mu,\nu} E_\mu H_\nu f_{\mu\nu}{}^{(11)} = \pm e \frac{\mathbf{v} \times \mathbf{H}}{c} \cdot \nabla_P (\pm e\tau \mathbf{E} \cdot \nabla_P f^{(0)})$$

whence

$$f_{\mu\nu}{}^{(11)} = \frac{e^2\tau}{c} \sum_{\alpha,\beta} \delta_{\nu\alpha\beta} v_\beta \frac{\partial}{\partial P_\alpha} \left(\tau \frac{\partial f^{(0)}}{\partial P_\mu} \right) \tag{33}$$

where $\delta_{\nu\alpha\beta} = 0$ if any two of its suffixes are the same, and ± 1 if the suffixes are an even (odd) permutation of xyz.

The physical meaning of the steps leading to (33) is just that a weak magnetic field perturbs the $f^{(1)}$ solution of Section 2 by displacing each part of the distribution in the direction of $\mathbf{v} \times \mathbf{H}$ in crystal momentum space, the displacement being proportional to $\mathbf{v} \times \mathbf{H}$ and to τ.

The term (33) in the distribution function gives rise to a contribution $\mathbf{j}^{(11)}$ to the current, which is at right angles to $\mathbf{H}$ and to $\mathbf{E}$. This contribution can be described by a "Hall conductivity tensor" $\sigma_{\lambda\mu\nu}$, thus:

$$j_\lambda{}^{(11)} = \sum_{\mu\nu} \sigma_{\lambda\mu\nu} E_\mu H_\nu \tag{34}$$

The contribution $\sigma_{\lambda\mu\nu}{}^{(i)}$ of the ith valley to $\sigma_{\lambda\mu\nu}$ is easily obtained from (33). We shall assume Maxwellian statistics, so that $\partial f^{(0)}/\partial P_\mu = -(v_\mu/kT) f^{(0)}$. When this is inserted into (33) the last factor involves a derivative of $v_\mu f^{(0)} \tau$ with respect to P_α. If τ depends only on energy, as we are assuming throughout this memorandum, the derivative of $f^{(0)}\tau$ with respect to P_α in (33) will be proportional to v_α, and $\Sigma_{\alpha,\beta} \delta_{\nu\alpha\beta} v_\beta v_\alpha$ will vanish identically because of the anti-symmetry of $\delta_{\nu\alpha\beta}$ in α and β. Therefore the only term which need be retained in $\partial/\partial P_\alpha$ is that in $\partial v_\mu/\partial P_\alpha$. If the coordinate axes are chosen along the principal axes of the energy surfaces of the ith valley, this latter derivative is just $\delta_{\mu\alpha}/m_\mu{}^*$. Thus we get, with the upper sign for n-type the lower for p,

$$\begin{aligned} \sigma_{\lambda\mu\nu}{}^{(i)} &= \mp \frac{e^3}{c} \sum_{\Delta \mathbf{P}^{(i)},s} \tau \sum_{\alpha,\beta} \delta_{\nu\alpha\beta} v_\lambda v_\beta \frac{\partial}{\partial P_\alpha} \left(- \frac{\tau f^{(0)} v_\mu}{kT} \right) \\ &= \pm \frac{e^3}{c} \sum_{\Delta \mathbf{P}^{(i)},s} \frac{\tau^2 f^{(0)}}{m_\mu{}^*} \sum_\beta \delta_{\nu\mu\beta} \frac{v_\lambda v_\beta}{kT} \end{aligned} \tag{35}$$

where as usual the first summation is over all vectors $\Delta \mathbf{P}^{(i)}$ in the ith

valley, per unit volume, and over both states of spin. In our present coordinate system the average of $v_\lambda v_\beta$ over an energy shell vanishes unless $\beta = \lambda$, while that of v_λ^2 can he evaluated from the equipartition relation (10): $v_\lambda^2 \to 2\Delta\epsilon/3m_\lambda^*$, where $\Delta\epsilon = |\epsilon - \epsilon_b|$ is the distance from the hand edge. Thus with $kT = \frac{2}{3}\langle\Delta\epsilon\rangle$, (35) reduces to

$$\sigma_{\lambda\mu\nu}^{(i)} = \mp \frac{e^3 n^{(i)}}{c} \frac{\langle\Delta\epsilon\tau^2\rangle}{\langle\Delta\epsilon\rangle} \frac{\delta_{\lambda\mu\nu}}{m_\lambda^* m_\mu^*} \tag{36}$$

where $n^{(i)}$, as in (9), is the number of carriers in the ith valley per unit volume, and where the angular hrackets are Maxwellian averages, as in (13).

The proportionality of the Hall conductivity tensor to $\langle\Delta\epsilon\tau^2\rangle$ and to the reciprocal product of two different principal masses is easy to understand physically. Without a magnetic field, an electric field in the μ direction gives a distribution, in each energy shell of the ith valley, which has a mean velocity in the μ direction proportional to $\Delta\epsilon\tau/m_\mu^*$ (cf. Section 2). Thus the distribution in this energy shell is acted on by a transverse magnetic force whose average value is proportional to this expression. This transverse magnetic force produces a transverse current proportional to the force and to τ/m_λ^*, where λ is the transverse direction.

For a cubic crystal the relation of the Hall current to $\mathbf{E}$ and $\mathbf{H}$ must be isotropic, i.e., the right of (34) must be proportional to $\mathbf{E} \times \mathbf{H}$. It is easily shown that the quantities in (34) are related to the ordinary conductivity σ_0, Hall coefficient R, and Hall mobility $\mu_H = R\sigma_0 c$, by

$$\mathbf{j}^{(11)} = \sigma_0^2 R\, \mathbf{E} \times \mathbf{H}$$

or

$$\sigma_{\lambda\mu\nu} = \sigma_0^2 R \delta_{\lambda\mu\nu} = \mp \frac{\sigma_0 \mu_H}{c} \delta_{\lambda\mu\nu} \tag{37}$$

where as usual the upper sign is for n-type, the lower for p. Since $\Sigma_{\lambda\mu\nu}\sigma_{\lambda\mu\nu}\delta_{\lambda\mu\nu}$ is invariant with respect to changes in the orientation of the coordinate system, we may evaluate it hy evaluating each $\Sigma_{\lambda\mu\nu}\sigma_{\lambda\mu\nu}{}^{(i)}\delta_{\lambda\mu\nu}$ in the system of principal axes of the ith valley, and then summing on i. From (36) we find in this way

$$\begin{aligned} \sigma_0^2 R = \mp \frac{\sigma_0 \mu_H}{c} &= \tfrac{1}{6} \sum_{\lambda\mu\nu} \sigma_{\lambda\mu\nu}\delta_{\lambda\mu\nu} = \tfrac{1}{6} \sum_i \sum_{\lambda\mu\nu} \sigma_{\lambda\mu\nu}{}^{(i)}\delta_{\lambda\mu\nu} \\ &= \mp \frac{e^3 n}{c} \frac{\langle\Delta\epsilon\tau^2\rangle}{\langle\Delta\epsilon\rangle} \cdot \tfrac{1}{3} \left(\frac{1}{m_1^* m_2^*} + \frac{1}{m_2^* m_3^*} + \frac{1}{m_3^* m_1^*} \right) \end{aligned} \tag{38}$$

where $n = \Sigma_i n^{(i)}$ is the total density of carriers. A neater way of pre-

TABLE III — VALUES OF THE LAST FACTOR IN (39), FOR CASES OF THE FORM

$$m_1^* = m_2^* = m_\perp^*,\ m_3^* = m_\parallel^*.$$

$\frac{m_\parallel^*}{m_\perp^*}$	$B = \frac{3\frac{m_\parallel^*}{m_\perp^*}\left(2 + \frac{m_\parallel^*}{m_\perp^*}\right)}{\left(1 + 2\frac{m_\parallel^*}{m_\perp^*}\right)^2}$
20	0.784
10	0.816
5	0.868
3	0.918
2	0.960
1	1.000
0.5	0.938
0.3	0.808
0.2	0.674
0.1	0.437
0.05	0.254

senting this result is in terms of the ratio μ_H/μ. Multiplying (38) by $c/\sigma_0\mu$ and using $\sigma_0 = ne\mu$ and (14) for μ we get

$$\frac{\mu_H}{\mu} = \frac{\langle\Delta\epsilon\tau^2\rangle\langle\Delta\epsilon\rangle}{\langle\Delta\epsilon\tau\rangle^2} \cdot \frac{3\left(\frac{1}{m_1^* m_2^*} + \frac{1}{m_2^* m_3^*} + \frac{1}{m_3^* m_1^*}\right)}{\left(\frac{1}{m_1^*} + \frac{1}{m_2^*} + \frac{1}{m_3^*}\right)^2} \tag{39}$$

$$= \frac{\langle\Delta\epsilon\tau^2\rangle\langle\Delta\epsilon\rangle}{\langle\Delta\epsilon\tau\rangle^2} \cdot B, \qquad \text{say.}$$

Note that the first factor of (39) is the value of μ_H/μ in the simple theory,[11] and that the second factor B, involving the anisotropy of the effective mass, is unity for zero anisotropy and <1 in general. Some sample values of this mass factor B are given in Table III and Fig. 7. Fig. 8 gives values of the first factor in (39), for the simplified model of intra- and inter-valley scattering described by (24).

7. THE BENEDICT-SHOCKLEY EXPERIMENT

We turn now to the response of the assembly of carriers to an electric field which varies sinusoidally with time. As Benedict and Shockley have shown,[12] this response becomes limited at high frequencies by the inertia of the carriers, and so by measuring it one can obtain an effective mass.

[11] See, for example, Reference 7, p. 277.
[12] T. S. Benedict and W. Shockley, Phys. Rev., **89**, p. 1152, 1953.

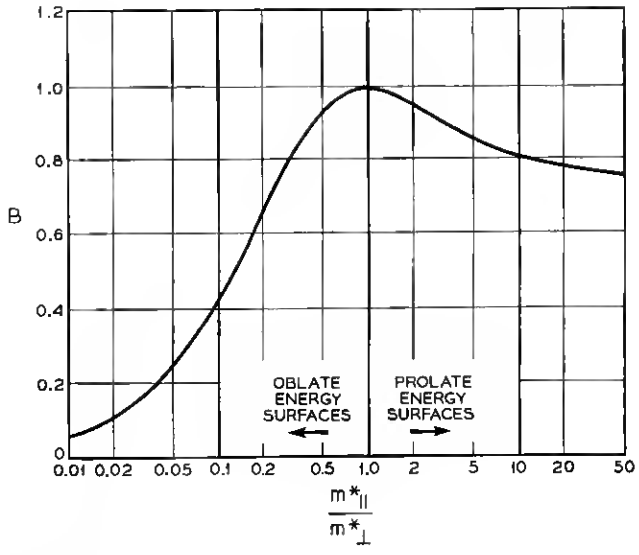

Fig. 7 — Dependence of

$$B = \frac{3\left(\frac{1}{m_1^* m_2^*} + \frac{1}{m_2^* m_3^*} + \frac{1}{m_3^* m_1^*}\right)}{\left(\frac{1}{m_1^*} + \frac{1}{m_2^*} + \frac{1}{m_3^*}\right)^2}$$

on the anisotropy of the effective mass, for the case $m_1^* = m_2^* = m_\perp^*$, $m_3^* = m_\parallel^*$.

The solution of the transport equation for this case proceeds almost exactly as in Section 2. We assume that the scattering of the carrier is described by a relaxation time τ, whose dependence on position in momentum space we shall for the moment leave unrestricted. The analysis starts as before from (3) for the distribution function f of the carriers, namely, with the upper sign for electrons, the lower for holes,

$$\frac{\partial f}{\partial t} = \pm e\mathbf{E}\cdot\nabla_P f - \frac{(f - f^{(0)})}{\tau} \tag{40}$$

(We neglect the very small effect of the magnetic field generated by $\partial\mathbf{E}/\partial t$.) Instead of (4) we write, if $\mathbf{E} = \mathbf{E}_0 e^{i\omega\tau}$,

$$f(t) = f^{(0)} + E_0\cdot\mathbf{f}^{(1)}(t) + O(E_0^2) \tag{41}$$

From (40) and (41) the equation for $f^{(1)}$ is

$$\frac{\partial \mathbf{f}^{(1)}}{\partial t} = \pm e\nabla_P f^{(0)} e^{i\omega t} - \frac{f^{(1)}}{\tau} \tag{42}$$

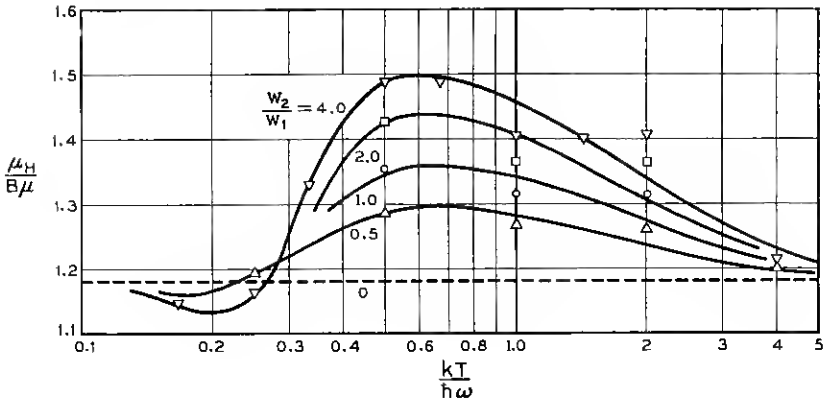

Fig. 8 — Values of the ratio

$$\frac{\mu_H}{B\mu} = \frac{\langle \Delta\epsilon\tau^2\rangle\langle\Delta\epsilon\rangle}{\langle\Delta\epsilon\tau\rangle^2},$$

for the simplified lattice scattering law (24). The ratio w_2/w_1 measures the strength of the coupling of the carriers to inter-valley modes in terms of that for intra-valley scattering; ω is the frequency of the inter-valley modes. The curves have been drawn to smooth out irregularities (severe for $kT/\hbar\omega = 1$ to 2) in the calculated points.

If $\Delta\epsilon = |\epsilon - \epsilon_b|$ is the distance from the band edge, we have, for Maxwellian statistics, $f^{(0)} \propto \exp(-\Delta\epsilon/kT)$ and of course $\nabla_P \Delta\epsilon = \mathbf{v}$, the group velocity. Thus $\mathbf{f}^{(1)} = f_0^{(1)} e^{i\omega t}$ with

$$\mathbf{f}_0^{(1)} = \frac{\mp e\mathbf{v} f^{(0)}\tau}{kT(1 + i\omega\tau)} \tag{43}$$

The current density is given by the usual sum over the different valleys i and the states ($\Delta\mathbf{P}^{(i)}$, spin) in each valley:

$$\mathbf{j} = \sum_i \sum_{\Delta\mathbf{P}^{(i)},s} (\mp e)\mathbf{v}(\Delta\mathbf{P}^{(i)}) f(\Delta\mathbf{P}^{(i)}) \tag{44}$$

From (41), (43) and (44),

$$\begin{aligned} \mathbf{j} &= \sum_i \sum_{\Delta\mathbf{P}^{(i)},s} \left(\frac{e^2\mathbf{v}\mathbf{v}\cdot\mathbf{E}_0 f^{(0)}\tau}{kT(1 + i\omega\tau)}\right) e^{i\omega\tau} \\ &= \frac{e^2\mathbf{E}_0}{3kT} \sum_i \sum_{\Delta\mathbf{P}^{(i)},s} \left(\frac{v^2 f^{(0)}\tau}{(1 + i\omega\tau)}\right) e^{i\omega\tau} \end{aligned} \tag{45}$$

if the crystal has cubic symmetry. Thus the semiconductor has the fre-

quency-dependent complex conductivity

$$\sigma(\omega) = \frac{ne^2}{3kT}\left\langle \frac{v^2\tau}{1 + i\omega\tau} \right\rangle \tag{46}$$

where n is the number of carriers per unit volume and the angular brackets denote a Maxwellian average. Note that in deriving (46) we have not had to assume anything about the dependence of ϵ or τ on $\Delta\mathbf{P}$; (46) is therefore valid for all models, not merely for the many-valley case. However, (46) is still not explicit enough to be directly usable for the evaluation of experimental results, and we shall need to use the special properties of the many-valley model to express the Maxwellian average in terms of measurable or readily interpretable quantities.

Under the usual assumptions of this paper τ is a function of energy ϵ only, so the average in (46) depends only on the average of v^2 over an energy shell. By the equipartition principle (10) we may therefore replace v^2 by

$$2\left(\frac{\frac{1}{2}m_1^*v_1^2}{m_1^*} + \frac{\frac{1}{2}m_2^*v_2^2}{m_2^*} + \frac{\frac{1}{2}m_3^*v_3^2}{m_3^*}\right) = \tfrac{2}{3}\Delta\epsilon\left(\frac{1}{m_1^*} + \frac{1}{m_2^*} + \frac{1}{m_3^*}\right) \tag{47}$$

The average of the masses is the same $m^{(I)}$ we encountered in Section 2, namely,

$$\frac{1}{m^{(I)}} = \tfrac{1}{3}\left(\frac{1}{m_1^*} + \frac{1}{m_2^*} + \frac{1}{m_3^*}\right) \tag{48}$$

Therefore

$$\left\langle \frac{v^2\tau}{1 + i\omega\tau} \right\rangle = \frac{2}{m^{(I)}}\left\langle \frac{\Delta\epsilon\tau}{1 + i\omega\tau} \right\rangle \tag{49}$$

The expression for $\sigma(\omega)$ becomes, with its real and imaginary parts separated,

$$\sigma(\omega) = \frac{2ne^2}{3kTm^{(I)}}\left[\left\langle \frac{\Delta\epsilon\tau}{1 + \omega^2\tau^2} \right\rangle - i\omega\left\langle \frac{\Delta\epsilon\tau^2}{1 + \omega^2\tau^2} \right\rangle\right] \tag{50}$$

The real part $\sigma_R(\omega)$ of this is what is usually called the "conductivity". The imaginary part $\sigma_I(\omega)$ is proportional to a contribution to the dielectric constant $\kappa(\omega)$, since $(4\pi)^{-1}\kappa(\omega)\partial\mathbf{E}/\partial t$ is the sum of the displacement current $(4\pi)^{-1}\kappa_0\partial\mathbf{E}/\partial t$ and the part of the true current j which is in phase with $\partial\mathbf{E}/\partial t$. Thus the departure of $\kappa(\omega)$ from the dielectric constant κ_0 of the crystal without its free carriers is given by

$$\kappa_0 - \kappa(\omega) = -\frac{4\pi}{\omega}\sigma_I(\omega) \tag{51}$$

At the frequencies and temperatures which have been used for the Benedict-Shockley experiment, most of the carriers have relaxation times short compared to ω^{-1}, and it is appropriate to make an expansion in powers of ω:

$$\left\langle \frac{\Delta\epsilon\tau}{1+\omega^2\tau^2} \right\rangle = \langle\Delta\epsilon\tau\rangle - \omega^2\langle\Delta\epsilon\tau^3\rangle \cdots \tag{52}$$

$$\left\langle \frac{\Delta\epsilon\tau^2}{1+\omega^2\tau^2} \right\rangle = \langle\Delta\epsilon\tau^2\rangle - \omega^2\langle\Delta\epsilon\tau^4\rangle \cdots \tag{53}$$

(If $\tau \to \infty$ as $\Delta P \to 0$, as would be the case if the only scattering were by phonons of negligible energy, the series (52), (53) do not converge for any finite ω. However, asymptotic series can be written down which differ only in order ω^3 and higher from the series obtained by simply expanding the denominators). Denoting the dc conductivity by σ_0 — equal to ne times the μ of (14) — we have from (50) to (53)

$$\sigma_R(\omega) = \sigma_0\left[1 - \frac{\omega^2\langle\Delta\epsilon\tau^3\rangle}{\langle\Delta\epsilon\tau\rangle} + O(\omega^4)\right] \tag{54}$$

$$\kappa_0 - \kappa(\omega) = 4\pi\sigma_0\left[\frac{\langle\Delta\epsilon\tau^2\rangle}{\langle\Delta\epsilon\tau\rangle} - \omega^2\frac{\langle\Delta\epsilon\tau^4\rangle}{\langle\Delta\epsilon\tau\rangle} + O(\omega^4)\right] \tag{55}$$

It is convenient to express the first term in the square bracket in (55) in terms of the Hall mobility μ_H, since the same average $\langle\Delta\epsilon\tau^2\rangle$ occurs in (38) as in (55). Let us set $\sigma_0 = ne\mu$ and use the designation B for the last factor in (39), a factor $\leqq 1$ dependent on the anisotropy of the effective mass in each valley and close to unity unless the anisotropy is very extreme (see Table III). Then

$$\kappa_0 - \kappa(\omega) = \frac{4\pi n\mu\mu_H m^{(I)}}{B}\left[1 - \omega^2\frac{m^{(I)2}\mu\mu_H}{e^2B}\frac{\langle\Delta\epsilon\tau^4\rangle\langle\Delta\epsilon\rangle}{\langle\Delta\epsilon\tau^2\rangle^2} + O(\omega^4)\right] \tag{56}$$

Equations (55) and (56), like all equations in this memorandum, is in Gaussian units. For rationalized MKS units, as used in the papers of Benedict and Shockley, the coefficient 4π should be replaced by $1/\epsilon_0$, where ϵ_0 is the permittivity of the vacuum.

The leading term of (56) is the same as that which one would obtain by simply replacing μ^2 by $\mu\mu_H/B$ in the formula used by Benedict and Shockley (simple model, τ = constant). But because the dimensionless factor $\langle\Delta\epsilon\tau^4\rangle\langle\Delta\epsilon\rangle/\langle\Delta\epsilon\tau^2\rangle^2$ is always $\geqq 1$ instead of $=1$, the second term in the brackets in (56) is not the same as that resulting from this substitution. Thus the expression used by Benedict[13] in his later analysis of data

[13] T. S. Benedict, Phys. Rev., **91**, p. 1565, 1953.

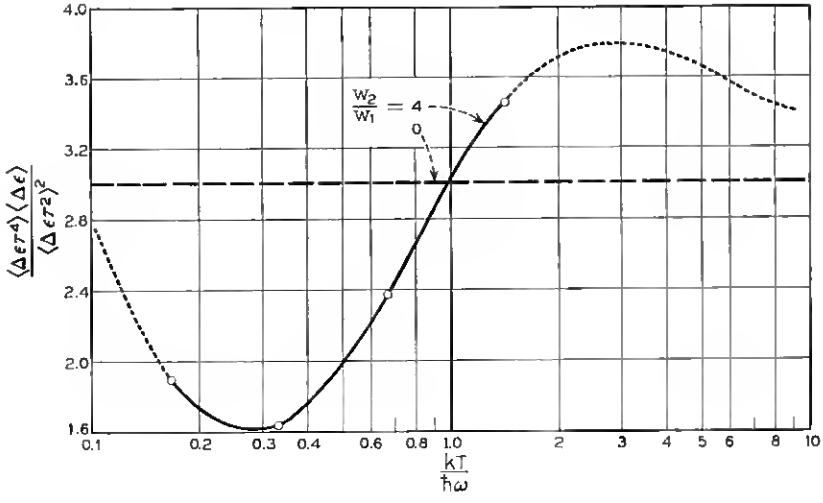

Fig. 9 — Sample values of the quantity $\frac{\langle\Delta\epsilon\tau^4\rangle\langle\Delta\epsilon\rangle}{\langle\Delta\epsilon\tau^2\rangle^2}$ occurring in the equation (56) for the high-frequency dielectric constant, for the simplified lattice scattering law (24). The ratio w_2/w_1 measures the strength of the coupling of the carriers to inter-valley modes in terms of that for intra-valley scattering; ω is the frequency of the inter-valley modes. The dotted extrapolations are qualitative only.

on p germanium is corrected only to the zeroth order in ω and to the approximation $B \approx 1$. Some sample values of the ratio $\langle\Delta\epsilon\tau^4\rangle\langle\Delta\epsilon\rangle/\langle\Delta\epsilon\tau^2\rangle^2$ have been computed for the scattering law (24), and are graphed in Fig. 9. These show that the range of possible variation of this factor is considerable.

A similar, though less useful, transformation can be made on (54), to express the second term in brackets in terms of the dimensionless coefficient G defined by

$$G = \frac{\langle\Delta\epsilon\tau^3\rangle\langle\Delta\epsilon\rangle^2}{\langle\Delta\epsilon\tau\rangle^3} \tag{57}$$

This is a coefficient which we shall encounter in the next section, in the theory of magnetoresistance, and which is graphed in Fig. 10 for the inter-valley scattering law (24). We find

$$\sigma_R(\omega) = \sigma_0\left[1 - \omega^2\frac{m^{(I)2}\mu^2}{e^2}G + O(\omega^4)\right] \tag{58}$$

The quantity G is $\geqq 1$, the equality holding only if τ is a constant. Table

IV and Fig. 10 give some typical values, for scattering laws of the form $\tau \propto \Delta\epsilon^r$ or of the form (24).

8. LOW-FIELD MAGNETORESISTANCE

In Section 6 we set up the Boltzmann equation for the steady motion of charge carriers under the combined influence of an electric field **E** and a magnetic field **H**, and solved it to the first order in H. We shall now undertake to solve this equation to the second and higher orders in H. The solution has been worked out independently for a number of cases by Abeles and Meiboom,[3] Shibuya,[3] and Shockley (unpublished). We shall not give all the details of the solution, especially at large H, as many of them can be found in the reference just mentioned. However, to emphasize some features not brought out in this previously published work we shall review the whole calculation briefly from the beginning.

The relation of theory and experiment in the area of magnetoresistance resembles that for piezoresistance, in that the tensor quantity which is

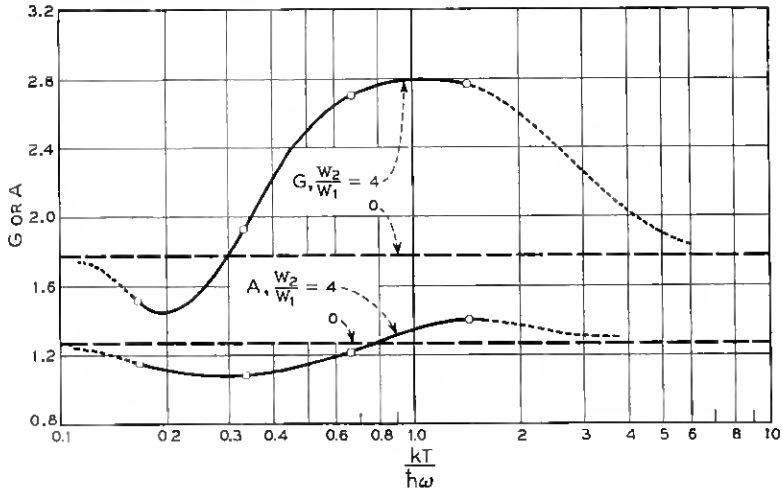

Fig. 10 — Sample values of

$$G = \frac{\langle \Delta\epsilon\tau^3\rangle\langle\Delta\epsilon\rangle^2}{\langle\Delta\epsilon\tau\rangle^3} \quad \text{and} \quad A = \frac{\langle\Delta\epsilon\tau^3\rangle\langle\Delta\epsilon\tau\rangle}{\langle\Delta\epsilon\tau^2\rangle^2}$$

for the simplified lattice scattering law (24). The ratio w_2/w_1 measures the strength of the coupling of the carriers to inter-valley modes in terms of that for intra-valley scattering; ω is the frequency of the inter-valley modes. The G curve has been drawn to be roughly consistent with the smoother A curve and the curve of Fig. 8. The dotted extrapolations of the curves are intended only to show the expected qualitative behavior.

TABLE IV — SAMPLE VALUES OF THE QUANTITIES G AND A DEFINED BY (57) AND (68), RESPECTIVELY

Scattering Law	$G = \frac{\langle \Delta\epsilon\tau^2\rangle \langle \Delta\epsilon\rangle^2}{\langle \Delta\epsilon\tau\rangle^3}$	$A = \frac{\langle \Delta\epsilon\tau^2\rangle \langle \Delta\epsilon\tau\rangle}{\langle \Delta\epsilon\tau^2\rangle^2}$
$\tau \propto \Delta\epsilon^{-0.5}$	2.58	4.01
$\tau \propto \Delta\epsilon^{-0.5}$	1.77	1.27
$\tau =$ constant	1.00	1.00
$\tau \propto \Delta\epsilon^{0.5}$	1.33	1.09
$\tau \propto \Delta\epsilon$	2.52	1.28
$\tau \propto \Delta\epsilon^{1.5}$	5.89	1.58
Form (24), $w_2/w_1 = 4$, $kT/\hbar\omega = 1.43$	2.77	1.40
0.667	2.70	1.21
0.333	1.92	1.08
0.167	1.52	1.15

simplest to calculate is reciprocal to the one which is directly measured. Thus one measures piezoresistance but calculates elastoresistance. Similarly the measured magnetoresistance is a change in the electric field $\mathbf{E}$ for given current, whereas the simplest quantity to calculate is the change of the current for given $\mathbf{E}$, i.e., the dependence of the conductivity tensor on $\mathbf{H}$. We shall see below that the neatest way of comparing theory and experiment, at least for small H, is to invert the observed magnetoresistivity tensor to get the magnetoconductivity tensor, and then compare the latter with theory.

The Boltzmann equation (30), from which we shall start, is

$$0 = \pm e\mathbf{E}\cdot\nabla_P f \pm e\,\frac{\mathbf{v}\times\mathbf{H}}{c}\cdot\nabla_P f - \frac{(f - f^{(0)})}{\tau} \tag{59}$$

where as before the upper sign is for electrons, the lower for holes, f is the distribution function of the carriers, $f^{(0)}$ the (Maxwellian) distribution in thermal equilibrium, $\mathbf{v} = \nabla_P\epsilon$ the group velocity. As in Section 2 we set

$$f = f^{(0)} + \mathbf{E}\cdot\mathbf{f}^{(1)} + O(E^2) \tag{60}$$

and neglect higher order terms in $\mathbf{E}$. The resulting equation for $\mathbf{f}^{(1)}$ can be written in the condensed form[14,15]

$$0 = \pm\tau e\nabla_P f^{(0)} \pm \tau\mathbf{H}\cdot\boldsymbol{\gamma}\mathbf{f}^{(1)} - \mathbf{f}^{(1)} \tag{61}$$

where

$$\boldsymbol{\gamma} = \frac{e}{c}\,\mathbf{v}\times\nabla_P \tag{62}$$

In the notation of Davis,[14] and Seitz,[15] $\gamma = (e/\hbar^2 c)\Omega$, while in the notation of Abeles and Meiboom,[3] $\gamma = (e/c)\Omega$. The solution of (61) can be expressed formally in terms of the reciprocal of the operator $(1 \pm \tau\mathbf{H}\cdot\boldsymbol{\gamma})$:

$$\mathbf{f}^{(1)} = \pm(1 \pm \tau\mathbf{H}\cdot\boldsymbol{\gamma})^{-1}\tau c\nabla_P f^{(0)} \tag{63}$$

If we set

$$(1 \pm \tau\mathbf{H}\cdot\boldsymbol{\gamma})^{-1} = 1 \mp \tau\mathbf{H}\cdot\boldsymbol{\gamma} + (\tau\mathbf{H}\cdot\boldsymbol{\gamma})(\tau\mathbf{H}\cdot\boldsymbol{\gamma})\cdots \tag{64}$$

we see that the leading term of (63) is just the solution (5) of Section 2 for $H = 0$, while the next is just the term (33) of Section 6. In other words, the series (64) corresponds to an iterative solution of (59). If we are interested only in the first few powers of H, this iterative solution is as simple as any; at high fields it is better to solve (61) explicitly in closed form, a procedure we shall outline in the next section.

The solution given by (63) and (64) of course applies for any dependence of the relaxation time τ and the energy ϵ on position $\mathbf{P}$ in crystal momentum space. However, we are here interested only in the case where, in each valley i, ϵ is a quadratic function of the components of $\Delta\mathbf{P} = \mathbf{P} - \mathbf{P}^{(i)}$ and where τ is a function of ϵ only. For this case some simplifications are possible. For one thing, τ commutes with the operator $\boldsymbol{\gamma}$, since (62) acting on a function of ϵ contains the factor $\mathbf{v} \times \nabla_P\epsilon \equiv 0$. The expression for the current density $\mathbf{j}$ in powers of H has the form

$$j_\mu = \sum_\nu \sigma_{\mu\nu}E_\nu + \sum_{\nu\alpha} \sigma_{\mu\nu\alpha}H_\alpha E_\nu + \sum_{\nu\alpha\beta} \sigma_{\mu\nu\alpha\beta}H_\alpha H_\beta E_\nu + \cdots \tag{65}$$

where of course $\sigma_{\mu\nu} = \sigma_0\delta_{\mu\nu}$ for a cubic substance, with σ_0 given by the equations of Section 2, and similarly $\sigma_{\mu\nu\alpha} = \sigma_0{}^2 R\delta_{\mu\nu\alpha}$, where R is the low-field Hall constant and as in Section 6 $\delta_{\mu\nu\alpha} = \pm 1$ if $\mu\nu\alpha$ is an even (odd) permutation of 123, zero otherwise. To get the contribution of the ith valley to the second-order "magnetoconductivity" tensor $\sigma_{\mu\nu\alpha\beta}$, we multiply (60) by $\pm ev_\mu$, insert (63) and (64), and sum on all momentum vectors in the ith valley and in unit volume, and on spins. The result is

$$\sigma_{\mu\nu\alpha\beta}{}^{(i)} = \frac{e^2}{kT} \sum_{\Delta\mathbf{P}^{(i)},s} f^{(0)}\tau^3(v_\mu\gamma_\alpha\gamma_\beta v_\nu)_{\text{symm}} \tag{66}$$

where as usual we have assumed $f^{(0)}$ to be Maxwellian, and where the subscript "symm" means that the expression in parentheses is to be averaged with the expressions obtained from it by permuting α with β, since only the part of $\sigma_{\mu\nu\alpha\beta}$ symmetrical in α and β has physical signifi-

[14] L. Davis, Phys. Rev., **56**, p. 93, 1939.
[15] F. Seitz, Phys. Rev., **79**, p. 372, 1950.

cance. (This symmetrization is not necessary, but simplifies the work by preventing the appearance of meaningless components.)

The explicit evaluation of (66) is a straightforward but tedious exercise in algebra, and will not be given in detail here. However, there are some important properties of the tensor (66) which can be established rather simply. Since the components of $\mathbf{v}$ are linear functions of the components of $\Delta\mathbf{P}$, the operator γ defined by (62) takes any linear function of the ΔP_λ into another linear function. Therefore the $v_\mu\gamma_\alpha\gamma_\beta v_\nu$ in (66) is a quadratic function of the ΔP_λ, and it is easily seen that this function contains denominators of the fourth degree in the effective masses. Now a quadratic function of the ΔP_λ can be written as an effective mass times the energy $\Delta\epsilon$ relative to the band edge, times a function of the direction of $\Delta\mathbf{P}$, dependent only on the ratios of the effective masses in the principal directions. Thus we may write, for example,

$$v_\mu\gamma_\alpha\gamma_\beta v_\nu = \frac{\Delta\epsilon}{m^{(I)3}} \times \text{function } (\mu\nu\alpha\beta, \text{ direction of } \Delta\mathbf{P}, \text{ mass ratios}) \quad (67)$$

where $m^{(I)}$ is the inertial average of the effective masses, defined by (15). Now let the summation on $\Delta\mathbf{P}$ be broken up into a summation over values in an energy shell $\Delta\epsilon$ to $\Delta\epsilon + d\Delta\epsilon$, and a summation over different shells. The function of direction in (67) will be the same for all the shells, and so we have the result

$$\sigma_{\mu\nu\alpha\beta}{}^{(i)} = \frac{a}{m^{(I)3}} F_{\mu\nu\alpha\beta}{}^{(i)}$$

where $F_{\mu\nu\alpha\beta}{}^{(i)}$ depends on the anistropy ratios of the effective masses in the ith valley, but not on the variation of τ with energy, while a is proportional to the number of carriers in the valley and to the Maxwellian average of $\tau^3\Delta\epsilon$.

It is convenient to express the average of $\tau^3\Delta\epsilon$ in dimensionless form by using the quantity G defined by (57), namely,

$$G = \frac{\langle\Delta\epsilon\tau^3\rangle\langle\Delta\epsilon\rangle^2}{\langle\Delta\epsilon\tau\rangle^3}$$

or else the quantity

$$A = \frac{\langle\Delta\epsilon\tau^3\rangle\langle\Delta\epsilon\tau\rangle}{\langle\Delta\epsilon\tau^2\rangle^2} \quad (68)$$

Here as usual the angular brackets denote Maxwellian averages as defined in connection with (14). We may use (14) to eliminate $m^{(I)}$ and the carrier density and if we wish we may eliminate μ in favor of μ_H by (39).

The result is

$$\sigma_{\mu\nu\alpha\beta}^{(i)} = G\frac{(\sigma_0\mu^2)}{(N_V c^2)} B^2 F_{\mu\nu\alpha\beta}^{(i)} = A\frac{(\sigma_0\mu_H^2)}{(N_V c^2)} F_{\mu\nu\alpha\beta}^{(i)} \tag{69}$$

where σ_0, μ, μ_H, are the conductivity, mobility, and Hall mobility, respectively, at $H = 0$, N_V is the number of valleys, and where $B \leqq 1$ is the function of the effective mass ratios defined in (39) and Table III. Summing on valleys i gives

$$\sigma_{\mu\nu\alpha\beta} = A\left(\sigma_0\frac{\mu_H^2}{c^2}\right) F_{\mu\nu\alpha\beta} = G\left(\sigma_0\frac{\mu^2}{c^2}\right) B^2 F_{\mu\nu\alpha\beta} \tag{70}$$

$$F_{\mu\nu\alpha\beta} = \frac{1}{N_V}\sum_i F_{\mu\nu\alpha\beta}^{(i)} \tag{71}$$

Note that $F_{\mu\nu\alpha\beta}$, as defined by (70) or (71), is dimensionless, as are G and A; $F_{\mu\nu\alpha\beta}$ or $B^2 F_{\mu\nu\alpha\beta}$ depends on the geometry of the valleys and the ratios of the principal masses of a valley. We shall see presently how the analysis of experimental data is facilitated by this decomposition of the magnetoconductivity into the product of a scalar factor depending on the behavior of τ and a tensor factor depending on the shape of the energy surfaces.

The quantity A defined by (68), like G, is $\geqq 1$, the equality holding only if τ is a constant. Some sample graphs of A and G are shown in Fig. 10, for scattering laws of the form (24), and some numerical values for this case and for $\tau \propto \Delta\epsilon^r$ are given in Table IV. Note that for the ideal case of intra-valley lattice scattering only, a case approximated in very pure material at moderately low T, $r = -1/2$ and $A = 4/\pi = 1.27$, $G = 9\pi/16 = 1.77$. Table V gives values of all the nonvanishing coefficients $F_{\mu\nu\alpha\beta}^{(i)}$ relative to a coordinate system oriented along the principal axes of a valley. The middle rows of Table VI give the $F_{\mu\nu\alpha\beta}$, relative to the crystal axes, for some of the simpler possible arrangements of valleys. The entries were obtained, of course, by comparing (69) or (70) with the results of explicit evaluations of (66). For completeness, Table V also gives the directional factors involved in the contribution $\sigma_{\mu\nu}^{(i)}$ of a single valley to the conductivity tensor $\sigma_{\mu\nu}$ in the absence of a magnetic field, and to the Hall conductivity tensor $\sigma_{\mu\nu\alpha}$ defined by (34) or (65). All these table entries are similar to those given by Abeles and Meiboom.[3] However, they have given the unsymmetrized $\sigma_{\mu\nu\alpha\beta}$ etc. for the cases $r = -1/2$ and $+3/2$, in terms of mean free path, absolute values of the masses, and carrier concentration; here we have given the symmetrized $\sigma_{\mu\nu\alpha\beta}$ etc. in terms of the directly observable σ_0 and μ_H, and for any $\tau(\Delta\epsilon)$.

TABLE V — ANISOTROPY FACTORS FOR CONDUCTION, HALL EFFECT, AND MAGNETORESISTANCE CONTRIBUTIONS FROM A SINGLE VALLEY

Phenomenon and Text Reference	Type of Valley	Tensor Component	Value	Relative Value
Conduction, (11)	Any	$\mu_{\alpha\beta}{}^{(i)}$		$\frac{\delta_{\alpha\beta}}{m_\alpha{}^*}$
Hall effect (36)	Any	$\sigma_{\lambda\mu\nu}{}^{(i)}$		$\frac{\delta_{\lambda\mu\nu}}{m_\lambda{}^* m_\mu{}^*}$
	$m_1{}^* = m_2{}^* = m_\perp{}^*$ $m_3{}^* = m_\parallel{}^*$	$\sigma_{123}{}^{(i)}$		$\frac{1}{m_\perp{}^{*2}}$
		$\sigma_{312}{}^{(i)} = \sigma_{231}{}^{(i)}$		$\frac{1}{m_\parallel{}^* m_\perp{}^*}$
Magnetoresistance, (69)	Any	$F_{\alpha\alpha\alpha\alpha}{}^{(i)}$	0	0
		$F_{\alpha\alpha\beta\beta}{}^{(i)}$ $(\beta \neq \alpha)$	$-\frac{3(m_1{}^* m_2{}^* + m_1{}^* m_3{}^* + m_2{}^* m_3{}^*) m_\beta{}^*}{(m_1{}^* + m_2{}^* + m_3{}^*)^2 m_\alpha{}^*}$	$-\frac{m_\beta{}^*}{m_\alpha{}^*}$
		$F_{\alpha\beta\alpha\beta}{}^{(i)} = F_{\alpha\beta\beta\alpha}{}^{(i)} (\beta \neq \alpha)$	$\frac{3}{2}\frac{(m_1{}^* m_2{}^* + m_1{}^* m_3{}^* + m_2{}^* m_3{}^*)}{(m_1{}^* + m_2{}^* + m_3{}^*)^2}$	$\frac{1}{2}$
	$m_1{}^* = m_2{}^* = m_\perp{}^*$ $m_3{}^* = m_\parallel{}^*$	$F_{1122}{}^{(i)}$	$-\frac{3(m_\perp{}^* + 2m_\parallel{}^*) m_\perp{}^*}{(m_\parallel{}^* + 2m_\perp{}^*)^2}$	-1
		$F_{1133}{}^{(i)} = F_{2233}{}^{(i)}$	$-\frac{3(m_\perp{}^* + 2m_\parallel{}^*) m_\parallel{}^*}{(m_\parallel{}^* + 2m_\perp{}^*)^2}$	$-\frac{m_\parallel{}^*}{m_\perp{}^*}$
		$F_{3311}{}^{(i)} = F_{3322}{}^{(i)}$	$-\frac{3(m_\perp{}^* + 2m_\parallel{}^*) m_\perp{}^{*2}}{(m_\parallel{}^* + 2m_\perp{}^*)^2 m_\parallel{}^*}$	$-\frac{m_\perp{}^*}{m_\parallel{}^*}$
		$F_{1212}{}^{(i)} = F_{1313}{}^{(i)} = F_{2323}{}^{(i)}$	$\frac{3}{2}\frac{(m_\perp{}^* + 2m_\parallel{}^*) m_\perp{}^*}{(m_\parallel{}^* + 2m_\perp{}^*)^2}$	$\frac{1}{2}$

TABLE VI — EXPRESSIONS FOR THE $F_{\mu\nu\alpha\beta}$ OF (70) IN TERMS OF THE MASS RATIOS, AND FOR THE $\sigma_{\mu\nu\alpha\beta}$ OF (65) IN TERMS OF THE EMPIRICAL MAGNETORESISTANCE CONSTANTS b, c, d, OF (74)

$\mu\nu\alpha\beta$	$\alpha\alpha\alpha\alpha$	$\alpha\alpha\beta\beta$	$\alpha\beta\alpha\beta$ or $\alpha\beta\beta\alpha$	Other
$F_{\mu\nu\alpha\beta}$, (100) valleys	0	$-\dfrac{\left(1+2\dfrac{m_{\parallel}^*}{m_{\perp}^*}\right)\left[1+\dfrac{m_{\parallel}^*}{m_{\perp}^*}+\left(\dfrac{m^*_{\parallel}}{m_{\perp}^*}\right)^2\right]}{\dfrac{m_{\parallel}^*}{m_{\perp}^*}\left(2+\dfrac{m_{\parallel}^*}{m_{\perp}^*}\right)^2}$	$\frac{3}{2}\dfrac{\left(1+2\dfrac{m_{\parallel}^*}{m_{\perp}^*}\right)}{\left(2+\dfrac{m_{\parallel}^*}{m_{\perp}^*}\right)^2}$	0
Relative value	0	$\left[\left(\dfrac{m_{\parallel}^*}{m_{\perp}^*}\right)^{-1}+1+\dfrac{m_{\parallel}^*}{m_{\perp}^*}\right]$	$\frac{3}{2}$	0
$F_{\mu\nu\alpha\beta}$, (111) valleys	$-\frac{2}{3}\dfrac{\left(\dfrac{m_{\parallel}^*}{m_{\perp}^*}-1\right)^2\left(1+\dfrac{2m_{\parallel}^*}{m_{\perp}^*}\right)}{\dfrac{m_{\parallel}^*}{m_{\perp}^*}\left(2+\dfrac{m_{\parallel}^*}{m_{\perp}^*}\right)^2}$	$-\frac{1}{3}\dfrac{\left(1+2\dfrac{m_{\parallel}^*}{m_{\perp}^*}\right)\left[2+5\dfrac{m_{\parallel}^*}{m_{\perp}^*}+2\left(\dfrac{m_{\parallel}^*}{m_{\perp}^*}\right)^2\right]}{\dfrac{m_{\parallel}^*}{m_{\perp}^*}\left(2+\dfrac{m_{\parallel}^*}{m_{\perp}^*}\right)^2}$	$\frac{1}{6}\dfrac{\left(1+2\dfrac{m_{\parallel}^*}{m_{\perp}^*}\right)\left[2+5\dfrac{m_{\parallel}^*}{m_{\perp}^*}+2\left(\dfrac{m_{\parallel}^*}{m_{\perp}^*}\right)^2\right]}{\dfrac{m_{\parallel}^*}{m_{\perp}^*}\left(2+\dfrac{m_{\parallel}^*}{m_{\perp}^*}\right)^2}$	0
Relative value	$-4\left(\dfrac{m_{\parallel}^*}{m_{\perp}^*}-1\right)^2$	$-2\left[2+5\dfrac{m_{\parallel}^*}{m_{\perp}^*}+2\left(\dfrac{m_{\parallel}^*}{m_{\perp}^*}\right)^2\right]$	$\left[2+5\dfrac{m_{\parallel}^*}{m_{\perp}^*}+2\left(\dfrac{m_{\parallel}^*}{m_{\perp}^*}\right)^2\right]$	0
$\dfrac{\sigma_{\mu\nu\alpha\beta}}{\sigma_0}$	$-(b+c+d)$	$-b-\left(\dfrac{\mu_H}{c}\right)^2$	$-\frac{1}{2}c+\frac{1}{2}\left(\dfrac{\mu_H}{c}\right)^2$	0

The coordinate axes are assumed oriented along the cubic axes of the crystal, and α, β represent any two *different* ones of the three directions x, y, z. In the last row of the table we have adhered to established notation at the cost of a double meaning for the letter c: in the expressions μ_H/c it is the velocity of light; elsewhere it is the magnetoresistance constant defined by (74).

The qualitative behavior of the entries in Table V is easily understandable. The components $F_{\alpha\alpha\alpha\alpha}{}^{(i)}$ refer to the longitudinal magnetoconductivity when both electric and magnetic fields are in one of the principal directions of the valley, the α direction. Since a magnetic field in such an α direction does not change the α component of the velocity of the carrier, this longitudinal magnetoconductivity must vanish:

$$F_{\alpha\alpha\alpha\alpha}{}^{(i)} = 0.$$

It is easily verified that, for our model, the principal directions of a valley are the only directions in which the longitudinal magnetoconductivity contribution vanishes. Since the relative longitudinal magnetoconductivity $\Delta\sigma/\sigma$ is necessarily $\leqq 0$, and for a cubic crystal is the negative of the relative longitudinal magnetoresistivity $\Delta\rho/\rho$, we can conclude that on our model the vanishing of the longitudinal magnetoresistance in any direction is possible, at least for cubic materials, only if the direction in question is a principal axis of all the valleys. It can further be shown, though we shall not give the details here, that lack of constancy of τ over an energy shell, far from upsetting this conclusion, merely makes it impossible for the longitudinal magnetoresistance to vanish in *any* direction.

The nonvanishing magnetoconductance effects can be described in terms of the current due to the force exerted by the magnetic field on the transverse Hall current. This current is proportional to the Hall current and inversely proportional to the effective mass — call it $m_J{}^*$ — in the direction normal to the Hall current and to **H**, this being the direction of the force producing the second-order current. The Hall current, as we have noted in Section 6, is proportional to the zero-order current, hence to the reciprocal of the effective mass $m_E{}^*$ in the direction of **E**, and to the reciprocal of the effective mass $m_{E\cdot H}{}^*$ in the direction normal to **E** and **H**.

To employ these ideas specifically, consider first the component $\sigma_{\alpha\alpha\beta\beta}{}^{(i)}$, which measures the change in current in the α direction produced by a magnetic field in the β direction. Here $m_E{}^* = m_\alpha{}^*$, $m_{E\cdot H}{}^* = m_\gamma{}^* (\gamma \neq \alpha, \beta)$, $m_J{}^* = m_\alpha{}^*$. Thus

$$\sigma_{\alpha\alpha\beta\beta}{}^{(i)} \propto -\frac{1}{m_\alpha{}^{*2} m_\gamma{}^*} \quad (\gamma \neq \alpha, \beta) \tag{72}$$

the minus sign coming in because the second-order current is in the direction opposite to **E**. When we insert the mass-dependence of $\sigma_0 \mu_H{}^2$ into (69) and combine with the $F_{\alpha\alpha\beta\beta}{}^{(i)}$ of Table V, we do in fact find that $\sigma_{\alpha\alpha\beta\beta}{}^{(i)}$ contains the masses only as indicated in (72). (The fact that

$F_{\alpha\alpha\beta\beta}^{(i)}$ depends on the masses in a much more complicated way is due to our choice of the defining equation for it, (69); we chose to write this equation so that it involved only the directly measurable quantities σ_0 and μ_H, and the dimensionless quantities A and $F_{\mu\gamma\alpha\beta}^{(i)}$. This choice is the most convenient one for comparisons with experiment, but is less simple conceptually than a choice giving the factor (72).) The remaining independent component, $F_{\alpha\beta\alpha\beta}^{(i)}$, may be analyzed similarly. It represents the second-order current in the α direction due to an $\mathbf{E}$ in the β direction and an $\mathbf{H}$ in the direction midway between α and β. Here $m_E^* = m_\beta^*$, $m_{E\cdot H}^* = m_\gamma^*(\gamma \neq \alpha, \beta)$, $m_J^* = m_\alpha^*$. The Hall current is weaker by $2^{1/2}$ than for the previous case, because of the 45° angle between $\mathbf{E}$ and $\mathbf{H}$, and since the force producing the second-order current is at 45° to the β direction, we must put a second $2^{1/2}$ in the denominator. Thus

$$\sigma_{\alpha\beta\alpha\beta}^{(i)} \propto \frac{1}{2m_\alpha^* m_\beta^* m_\gamma^*} = \frac{1}{2m_1^* m_2^* m_3^*} \tag{73}$$

This, again, can be verified to follow from (69) and Table V.

To apply these results to experimental magnetoresistance data in the region of proportionality to H^2, it is necessary, as has been mentioned above, to derive an experimental magnetoconductivity tensor from the observed magnetoresistance. For a cubic crystal the magnetoresistivity tensor can be described by three constants b, c (not to be confused with velocity of light), d, defined by

$$\frac{\Delta\rho}{\rho H^2} = bH^2 + c\frac{(\mathbf{j}\cdot\mathbf{H})^2}{j^2} + d\frac{(j_x^2H_x^2 + j_y^2H_y^2 + j_z^2H_z^2)}{j^2} \tag{74}$$

where $\Delta\rho$ is the change of resistivity ρ due to a small field $\mathbf{H}$, and where the axes are those of the crystal. The equations relating the constants b, c, d to the corresponding constants describing the magnetoconductivity tensor have been given by Pearson and Suhl.[16] From these equations the components of $\sigma_{\mu\nu\alpha\beta}$ can be expressed in terms of the empirical constants b, c, d. The results are tabulated in the last row of Table VI.

If the ratios of these components are compared with the ratios of the corresponding $F_{\mu\nu\alpha\beta}$, one can check the correctness of an assumed model and determine the ratio $m_\parallel^*/m_\perp^*$. From the absolute values of the $\sigma_{\mu\nu\alpha\beta}$ one can then determine A. A further check is provided if data are available at more than one temperature, since the mass ratio should come out roughly independent of T, while the variation of A with T should

[16] G. L. Pearson and H. Suhl, Phys. Rev., **83**, p. 768, 1951.

accord with a reasonable picture of the effects of impurity, inter-, and intra-valley scattering on the form of $\tau(\Delta\epsilon)$.

An analysis of this sort has been carried out for n type silicon.[17] For this substance the longitudinal magnetoresistance nearly vanishes in directions of the type (100). From what has been said above, this almost requires that the band structure have valleys on the (100) axes in **K**-space, and that the relaxation time be practically a function of energy only. Fitting the remaining magnetoconductivity constants gives $m_{\parallel}^*/m_{\perp}^* \approx 5$; this ratio comes out independent of temperature as it should. It agrees with the ratio determined by cyclotron resonance.[18]

9. HALL EFFECT AND MAGNETORESISTANCE FOR LARGE MAGNETIC FIELDS

As the theory of Hall and magnetoresistance effects for large magnetic fields is rather complicated mathematically, it will suffice for our purposes merely to outline the approach which can be used and to quote a few results without proof. Some of the details can be found in the papers of Abeles and Meiboom[3] and of Shibuya.[3]

To treat these we solve the transport equation (61) for the distribution function $\mathbf{f}^{(1)}$ and calculate the current density from $\mathbf{f}^{(1)}$. This gives the electrical conductivity tensor $\sigma_{\mu\nu}(\mathbf{H})$, which can be inverted to give the resistivity tensor $\rho_{\mu\nu}$. The antisymmetric part of $\rho_{\mu\nu}$ determines a Hall coefficient (in general slightly orientation-dependent), and the symmetrical part determines the magnetoresistance.

The solution of (61) can be carried out either by summing the series (64), or directly by guessing that $\mathbf{f}^{(1)}$ will be a linear function of the velocity components, with coefficients which are functions of energy. These coefficients can be determined by solving a set of three simultaneous equations.

As $H \to \infty$, the conductivity tensor $\sigma_{\mu\nu}(\mathbf{H})$ becomes singular, the contribution $\sigma_{\mu\nu}^{(i)}$ of the ith valley taking the form

$$\sigma_{\mu\nu}^{(i)} \to \frac{ne^2}{N_V}\frac{\langle\Delta\epsilon\tau\rangle}{\langle\Delta\epsilon\rangle}\frac{H_\mu H_\nu}{m_1^* H_1^2 + m_2^* H_2^2 + m_3^* H_3^2} \qquad \text{in general}$$
$$= \frac{\sigma_0}{N_V}\frac{m^{(I)} H_\mu H_\nu}{m_1^* H_1^2 + m_2^* H_2^2 + m_3^* H_3^2} \qquad \text{for a cubic crystal} \tag{75}$$

where n is the total density of carriers, N_V the number of valleys, $\Delta\epsilon$ the distance from the band edge, $\tau(\Delta\epsilon)$ the relaxation time, σ_0 the conductivity at $H = 0$, $m^{(I)}$ the average inertial mass defined by (15), and

[17] G. L. Pearson and C. Herring, Physica, to appear.
[18] Dexter, Lax, Kip, and Dresselhaus, see Reference 5.

H_1, H_2, H_3 are the components of $\mathbf{H}$ along the principal axes of the valley. Summing (75) on i gives a limiting $\sigma_{\mu\nu}$ which is still proportional to $H_\mu H_\nu$; its determinant therefore vanishes, and it cannot be inverted to give the limiting $\rho_{\mu\nu}$. It turns out that (75) suffices to give the limiting value of the longitudinal magnetoresistance as $H \to \infty$, but that to get the limiting value of the transverse magnetoresistance it is necessary to evaluate contributions to $\sigma_{\mu\nu}(\mathbf{H})$ of order $1/H^2$. The limiting Hall coefficient can be obtained from the contributions of order $1/H$ to $\sigma_{\mu\nu}(\mathbf{H})$.

The following points are noteworthy: (i) The limiting value of the Hall coefficient as $H \to \infty$ is $R = \mp(1/nec)$, independently of the arrangement and mass anisotropy of the valleys, and of the dependence of τ on energy. Even if τ is not a mere function of energy, the same limiting form obtains. (ii) For $\mathbf{E}$ parallel to $\mathbf{H}$, the ratio $\sigma(H \to \infty)/\sigma_0$ depends on the arrangement and mass anisotropy of the valleys, but not on the law of variation of τ with energy, as long as τ is a function of energy only. (iii) For $\mathbf{E}$ not parallel to $\mathbf{H}$, both $\sigma(H \to \infty)$ and $\sigma(H \to \infty)/\sigma_0$ depend on the behavior of $\tau(\Delta\epsilon)$ as well as on the band structure.

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Appendix A

THE RELAXATION TIME ASSUMPTION

The use of the relaxation time concept represents a great simplification of the Boltzmann equation for all kinds of transport phenomena. To be strictly correct, one ought to describe the scattering processes which the carriers undergo by a transition probability $S(\mathbf{K}, \mathbf{K}')$ defined as the probability per unit time of a transition from an initial state $\mathbf{K}$ to a final state in unit volume of wave number space centered on $\mathbf{K}'$. (Conservation of energy will usually limit these transitions to a certain surface in $\mathbf{K}'$-space, so that S will contain a delta function of energy; however, this complica-

tion has no bearing on the remarks of this paragraph.) The Boltzmann equation, for the case of Maxwellian statistics, therefore takes the form

$$\frac{\partial f(\mathbf{K})}{\partial t} = \left(\frac{\partial f(\mathbf{K})}{\partial t}\right)_{\text{Fields}} + \int [f(\mathbf{K}')S(\mathbf{K}', \mathbf{K}) - f(\mathbf{K})S(\mathbf{K}, \mathbf{K}')]\, d\mathbf{K}'. \quad \text{(A1)}$$

This is in general an integral equation for the distribution function f, or for the part $\mathbf{E}\cdot\mathbf{f}^{(1)}$ of f which is linear in the electric field. Our task in this Appendix is to say a few words about the validity of approximating (A1) by an equation of the form

$$\frac{\partial f(\mathbf{K})}{\partial t} = \left(\frac{\partial f(\mathbf{K})}{\partial t}\right)_{\text{Fields}} - \left(\frac{f(\mathbf{K}) - f^{(0)}(\mathbf{K})}{\tau(\mathbf{K})}\right) \quad \text{(A2)}$$

and to examine the validity of the further approximation $\tau(\mathbf{K}) = \tau(\epsilon)$. We shall give only a rather brief discussion of these questions, however, as a future publication[6] will give a more thorough treatment and include a discussion of the solution of (A1) when these approximations fail.

To begin with, let us consider the special class of cases for which

$$S(\mathbf{K}', \mathbf{K}) = S(\mathbf{K}', \mathbf{K}^*) \quad \text{(A3)}$$

where $\mathbf{K}^*$ is the state in the same valley as $\mathbf{K}$ but with opposite velocity. If (4) is inserted for f in the integral of (A1), the $f^{(0)}$ term contributes nothing, and if (A3) is satisfied

$$\int \mathbf{E}\cdot\mathbf{f}^{(1)}(\mathbf{K}')S(\mathbf{K}', \mathbf{K})\, d\mathbf{K}' = 0, \quad \text{(A4)}$$

since $\mathbf{f}^{(1)}$ is an odd function of velocity while S is even. Therefore, to the first order in E, (A1) reduces to (A2) with

$$1/\tau(\mathbf{K}) = \int S(\mathbf{K}, \mathbf{K}')\, d\mathbf{K}' \quad \text{(A5)}$$

For collision processes which do not satisfy the velocity-randomizing condition (A3) we may assess roughly the legitimacy of using a $\tau(\epsilon)$ by comparing, for different initial states on the same constant energy surface, the mean rate with which scattering destroys the component of velocity in the original direction. This rate of loss of velocity defines a $1/\tau$ which if isotropic is known to be usable in (A2) for energy-conserving scattering processes in the simple model,[19] and for the many-valley model it is a reasonable presumption, borne out by the more rigorous treatment

[19] W. Shockley, *Electrons and Holes in Semiconductors* (Van Nostrand 1951) p. 251 et seq.

of Reference 6, that if this rate of loss of velocity is nearly constant over an energy surface, then (A2) is legitimate with $\tau = \tau(\epsilon)$.

We shall consider five types of scattering in turn, three by phonons and two by impurities. For the phonon processes, scattering of a carrier from $\mathbf{K}$ to $\mathbf{K}'$ involves absorption of a phonon of wave vector $\mathbf{K}' - \mathbf{K}$, or emission of one with the negative wave vector. The matrix element for such a process is of the form[20]

$$M(\mathbf{K}, \mathbf{K}') = \left.\begin{matrix} N^{1/2} \\ (N+1)^{1/2} \end{matrix}\right\} \frac{C(\mathbf{K}, \mathbf{K}')}{\omega^{1/2}} \text{ for} \left\{\begin{matrix} \text{absorption} \\ \\ \text{emission} \end{matrix}\right. \tag{A6}$$

where N is the occupation number of the lattice mode involved, ω is its frequency, and $C(\mathbf{K}, \mathbf{K}')$ is proportional to the matrix element, between states $\mathbf{K}$ and $\mathbf{K}'$, of the perturbation of the electronic Hamiltonian due to a static displacement of the nuclei of the lattice, of unit amplitude in this mode. The scattering function $S(\mathbf{K}, \mathbf{K}')$ which we have used above is given by

$$S(\mathbf{K}, \mathbf{K}') = \frac{2\pi}{\hbar} \sum | M(\mathbf{K}, \mathbf{K}') |^2 \delta[\epsilon(\mathbf{K}) - \epsilon(\mathbf{K}') \pm \hbar\omega] \tag{A7}$$

where δ is the Dirac delta function and the summation is over absorption (upper sign) and emission (lower sign), and over the various branches of the vibrational spectrum.

(i) *Inter-Valley Lattice Scattering.* Here the magnitude of $\mathbf{K}' - \mathbf{K}$ is large compared with the distance of either $\mathbf{K}$ or $\mathbf{K}'$ from the band edge point nearest it. Moreover, the total change in $\hbar\omega$ as $\mathbf{K}$ or $\mathbf{K}'$ ranges over a constant energy surface will be $\ll kT$ if the energy relative to the band edge is $\sim kT$. Therefore the percentage variation of $M(\mathbf{K}, \mathbf{K}')$ over such an energy surface will be small. And unless the energy relative to the band edge is extremely small, the surface in $\mathbf{K}'$-space which makes the argument of the delta function vanish will be nearly a constant energy surface. We conclude that $S(\mathbf{K}, \mathbf{K}')$ can be taken to be independent of $\mathbf{K}$ and $\mathbf{K}'$ when either ranges over a constant energy surface in its valley, and in particular, (A3) applies. Therefore inter-valley lattice scattering is described by a relaxation time which is given by (A5) and is a function of energy only.

(ii) *Intra-Valley Scattering by Optical Modes.* For a nonpolar crystal this case is essentially the same as the preceding, since the matrix element $C(\mathbf{K}, \mathbf{K}')$ is substantially equal to its limiting value as $\mathbf{K}' \to \mathbf{K}$. For a polar material the longitudinal polar optical modes give a $C(\mathbf{K}, \mathbf{K}') \propto$

[20] See, for example, Reference 19, p. 520.

$|\mathbf{K}' - \mathbf{K}|^{-1}$. In a cubic crystal this contribution is independent of the direction of $(\mathbf{K}' - \mathbf{K})$, but if the energy surfaces are anisotropic the variation of $C(\mathbf{K}, \mathbf{K}')$ with $|\mathbf{K}' - \mathbf{K}|$ will suffice to prevent $\tau(\mathbf{K})$ from being constant over an energy surface.

(iii) *Intra-Valley Scattering by Acoustical Modes.* Here (A6) and (A7) again apply, but with the simplification that for all but extremely slow carriers the $\hbar\omega$ in the argument of the delta function can be neglected, since only very low-energy phonons are involved. However, $C(\mathbf{K}, \mathbf{K}')$ need no longer be independent of direction. The reason for this is that according to the deformation potential concept,[21] C depends on the strain associated with the lattice mode in question. If only the volume dilatation affected C, as was the case for the simple model, C would be independent of the direction of the phonon wave vector $(\mathbf{K} - \mathbf{K}')$, since the dilatation amplitude in a compressional wave of unit displacement amplitude is independent of direction. But for a many-valley model both shears and dilatations can produce deformation potentials, and the nature of the shear strain in a shear wave of unit amplitude depends strongly on the direction of propagation. Therefore C may be a function of the direction of $(\mathbf{K} - \mathbf{K}')$, in any particular valley.

For a valley whose $\mathbf{K}^{(i)}$ lies on a threefold or fourfold symmetry axis of a crystal the deformation potentials due to the different possible types of strains can be expressed in terms of two constants, Ξ_d, Ξ_u, which appear in the theory of piezoresistance, Eq. (C6) below, and which are defined thus: Let $u_r (r = 1 \text{ to } 6)$ be the six components of the strain tensor, relative to the principal axes of the valley, the z axis being taken along the symmetry axis of the valley. Then a dilatation in the two directions normal to the symmetry axis $(u_1 = u_2 = u/2, u_3 = 0)$ produces a band edge shift $\Xi_d u$. A uniaxial shear $(u_1 = u_2 = -u/2, u_3 = u)$ produces a shift $\Xi_u u$. As will be shown in detail in Reference 6, it is not hard to evaluate the dependence of $C(\mathbf{K}, \mathbf{K}')$ on the direction of $\mathbf{K}' - \mathbf{K}$, in terms of Ξ_d and Ξ_u and the elastic constants of the crystal. Thus we can calculate the variation of $S(\mathbf{K}, \mathbf{K}')$ over an energy surface by (A7), in terms of the constants Ξ_d, Ξ_u, and the anisotropy of the effective mass.

We shall presently exhibit the results of some calculations, made by the procedure just outlined, of how much the rate of loss of initial velocity varies over an energy surface. However, we shall first present an argument that for given deformation potentials, the greatest variation of this quantity may be expected to occur for spherical energy surfaces,

[21] See, for example, Reference 19, p. 520 et seq.

and that usually very little variation will occur for extremely prolate or oblate surfaces. In other words, for almost all values of Ξ_d and Ξ_u, the use of a $\tau(\epsilon)$ will be justified for very prolate or very oblate surfaces. Fig. 11 shows the argument. In (a) is shown a spherical energy surface centered on a band edge point on some symmetry axis in **K**-space. We expect the greatest difference in relaxation time $\tau(\mathbf{K})$, defined in terms of rate of loss of initial velocity, to be that between a point $\mathbf{K}_1$ where the symmetry axis cuts the sphere and a point $\mathbf{K}_2$ 90° around the sphere from $\mathbf{K}_1$. Backward scattering processes for $\mathbf{K}_1$, i.e., those which almost reverse its velocity, have $\mathbf{K}' - \mathbf{K}_1$ vectors almost parallel to the symmetry axis, while forward scattering processes, which take $\mathbf{K}_1$ to a state $\mathbf{K}'$ with almost the same velocity, have $\mathbf{K}' - \mathbf{K}_1$ almost at right angles to the axis. For a carrier initially at $\mathbf{K}_2$, on the other hand, the vector $\mathbf{K}' - \mathbf{K}_2$ is almost perpendicular to the axis for backward scattering, while for forward scattering it may range from almost parallel (plane of paper) to perpendicular (normal to paper). For this case, therefore, a dependence of the scattering function on the inclination to the symmetry axis will be quite effective in producing an anisotropy of $\tau(\mathbf{K})$. Now consider the situation for a very prolate energy surface, as shown in (b) of Fig. 11. This figure has been derived from that of (a) by a horizontal extension and a vertical contraction. Now all the dotted lines representing vectors $\mathbf{K}' - \mathbf{K}_1$ or $\mathbf{K}' - \mathbf{K}_2$ are nearly parallel to the symmetry axis, and the

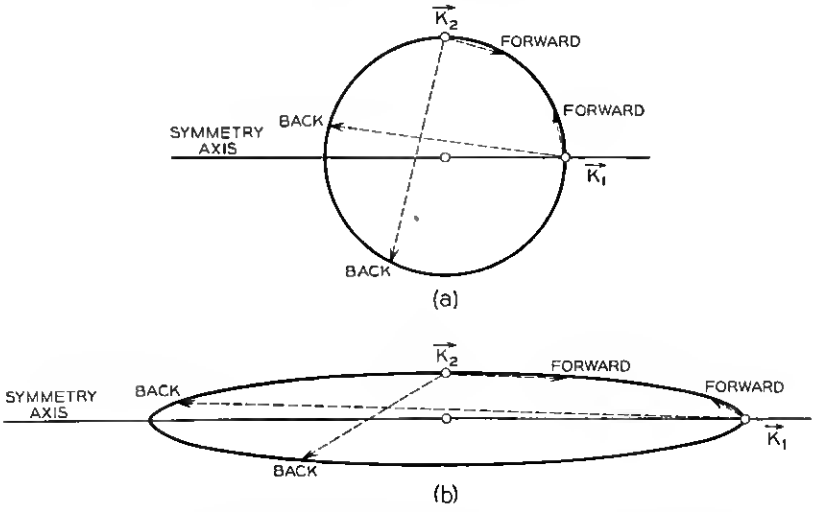

Fig. 11 — Comparison of intra-valley lattice scattering processes for a valley with spherical energy surfaces, (a), and a valley with highly prolate surfaces, (b).

corresponding scattering functions must therefore be very nearly the same. Of course, forward scattering from $\mathbf{K}_1$ through sufficiently small angles has $\mathbf{K}' - \mathbf{K}_1$ nearly normal to the axis, and the same is true for backward scattering from $\mathbf{K}_2$ in a small range close to 180°. But it is clear that as the energy surface becomes more prolate these cases form a smaller and smaller fraction of the total of possible final states $\mathbf{K}'$. Thus for extreme prolateness $\tau(\mathbf{K}_1) \to \tau(\mathbf{K}_2)$. For strongly oblate energy surfaces most of the $\mathbf{K}' - \mathbf{K}$ vectors approach normality to the symmetry axis, and a similar conclusion holds. The argument fails if, and only if, the scattering probability practically vanishes for $\mathbf{K}' - \mathbf{K}$ along the symmetry axis (prolate case) or perpendicular to it (oblate case).

Fig. 12 shows the results of some calculations of $\tau(\mathbf{K}_2)/\tau(\mathbf{K}_1)$ carried out by *E.* Vogt for the worst case, that of spherical energy surfaces, and for an actual case, that of valleys on a (111) axis with $m_\parallel^*/m_\perp^* = 1.3/.08$, the value found in cyclotron resonance experiments on *n* germanium.[5] The anisotropy of the elastic constants has been assumed to be that for germanium. For the spherical surfaces calculations were made for valleys centered on (100) and (111) axes, but the results were found to be indistinguishable. A comparison of the full curve (spherical surfaces) with the dashed one (prolate surfaces) shows, as expected, that with a highly anisotropic effective mass the anisotropy of the relaxation time is much less than for the spherical case, except near the ratio $\Xi_d/\Xi_u = -1$. This is the ratio for which modes with wave vectors along the symmetry axis are incapable of scattering. We conclude that for intra-valley lattice scattering the assumption of a relaxation time dependent only on energy will fail over a considerable range of the deformation potential parameters if the effective mass is isotropic, but only over a moderate range near $\Xi_d/\Xi_u = -1$ if the effective mass is very anisotropic.

(iv) *Scattering by Ionized Impurities.* To date the quantum theory of this effect has been developed only on the crude basis of treating the fluctuations of potential due to a random arrangement of ions as a small perturbation on the motion of the charge carriers.[22] The result is that the effective matrix element for scattering between two states $\mathbf{K}, \mathbf{K}'$ on the same energy surface is a function of $|\mathbf{K}' - \mathbf{K}|$ which is sharply peaked at very small values of this quantity, at least when the density of impurities is not too high. This means that the principal effects come from small-angle scattering, a fact well known in the classical theory of impurity

[22] H. Brooks, Phys. Rev., **83**, p. 8 & 9, 1951 (contains typographical errors); C. Horie, Tôh. U. Sci. Rep. **34**, 27 (1950); and C. Herring, unpublished.

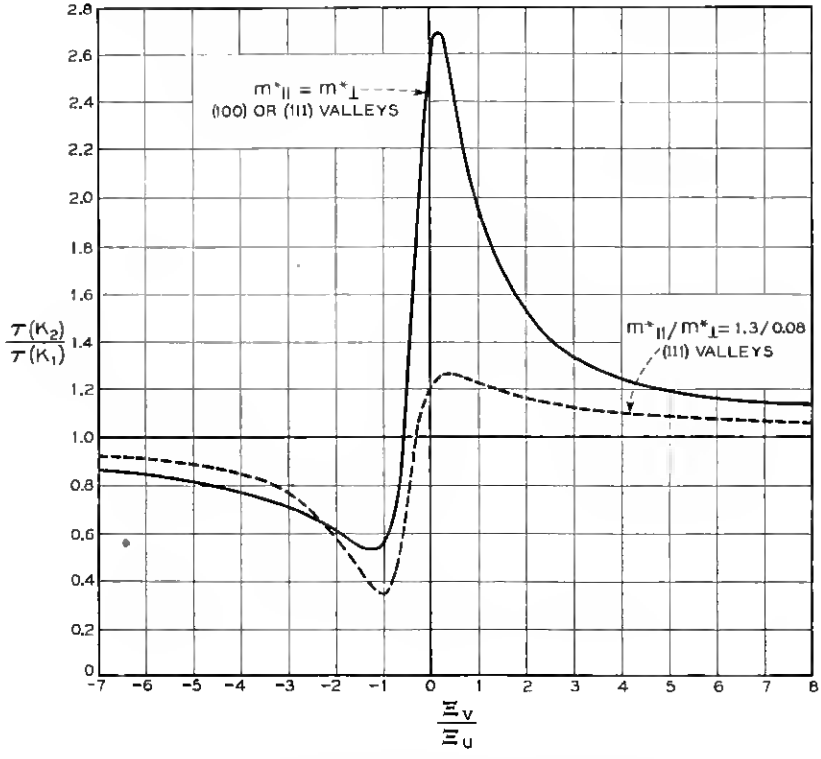

Fig. 12 — Anisotropy of the relaxation time for intra-valley lattice scattering, as a function of the ratio of the deformation potential coefficient Ξ_d for two-dimensional dilatation to the coefficient Ξ_u for uniaxial shear, as these quantities are defined in Appendix A or in Equation (C6). The ordinate is the ratio, for the points $\mathbf{K}_2$ and $\mathbf{K}_1$ of Fig. 11, of the effective relaxation time τ defined by $\tau^{-1} =$ — (initial velocity)$^{-1}$ (time rate of change of mean velocity, due to scattering). The elastic anisotropy assumed is that for germanium.

scattering.[23] Now the probability of a collision with a given range of $|\mathbf{K}' - \mathbf{K}|$ is proportional to the square of this matrix element and to the number of possible final states $\mathbf{K}'$ within the given range of distances from $\mathbf{K}$ and in a given small range of energy. A little calculation shows that this number is greater when $\mathbf{K}$ is near the $\mathbf{K}_1$ of Fig. 11(b) than when $\mathbf{K}$ is near $\mathbf{K}_2$. Moreover, the fractional loss of the velocity component in the initial direction is greater for a collision at $\mathbf{K}_1$ than at $\mathbf{K}_2$. The result

[23] E. Conwell and V. F. Weisskopf, Phys. Rev., **77**, p. 388, 1950; R. S. Cohen, L. Spitzer, Jr., and P. M. Routly, Phys. Rev., **80**, p. 230, 1950; and L. Spitzer, Jr. and R. Härm, Phys. Rev., **89**, p. 977, 1953.

is that carriers near $\mathbf{K}_1$ have a much shorter effective relaxation time for impurity scattering than do those near $\mathbf{K}_2$.

Thus if the energy surfaces are very anisotropic, the assumption $\tau = \tau(\epsilon)$ may be expected to be a poor approximation when ionized impurity scattering is important.

(v) *Neutral Impurity Scattering.* In the simple theory the scattering of charge carriers from neutral impurities in hydrogen-like states is mathematically equivalent to the scattering of electrons from hydrogen atoms.[24] At the temperatures at which such scattering is important the wavelength of the incident carrier is usually $\gg$ the diameter of the wave function of the center, so s wave scattering predominates. Therefore the scattering is isotropic. For a many-valley model, however, the situation seems at first sight more complicated, since the effective mass is anisotropic, and the centers are not spherically symmetrical. However, it can be shown[6] that, at least if the energy of the carrier is low enough, the scattered wave must be describable as an s wave in the space of the transformed coordinates defined by

$$\xi_\lambda = m_\lambda^{*\,1/2} x_\lambda \tag{A8}$$

In the corresponding momentum space (the φ-space of Appendix B) the surfaces of constant energy are spheres. It follows, that, at least at low energies, neutral impurity scattering satisfies (A3) and is describable by a constant relaxation time.

Appendix B

Equality of the Energy-Shell Averages

$$\tfrac{1}{2}\overline{m_1^* v_1^2}, \qquad \tfrac{1}{2}\overline{m_2^* v_2^2}, \qquad \tfrac{1}{2}\overline{m_3^* v_3^2}$$

Choose coordinate axes along the principal axes of the energy surfaces in any given valley. For $\lambda = 1, 2, 3$, let

$$\varphi_\lambda = v_\lambda (m_\lambda^*)^{1/2} = \Delta P_\lambda / (m_\lambda^*)^{1/2} \tag{B1}$$

Then

$$\Delta\epsilon \equiv |\, \epsilon(\Delta \mathbf{P}) - \epsilon_0 \,| = \tfrac{1}{2} \sum \varphi_\lambda^2 \tag{B2}$$

so that the energy surfaces are concentric spheres in φ-space. The density of φ-vectors consistent with the periodic boundary conditions is of course uniform, like that of $\Delta\mathbf{P}$. The average of $\tfrac{1}{2} m_\lambda^* v_\lambda^2$ over an energy shell is therefore the average of φ_λ^2 over a spherical shell, and thus obviously independent of λ.

[24] C. Erginsoy, Phys. Rev., **79**, p. 1013, 1950.

Appendix C

Explicit Calculation of Elastoresistance Constants

Let $\sigma_{\mu\nu}$ be the conductivity tensor of a crystal, defined by the relation

$$j_\mu = \sum_\nu \sigma_{\mu\nu} E_\nu \tag{C1}$$

between current density $\mathbf{j}$ and electric field $\mathbf{E}$. Let $u_{\alpha\beta}$ be the strain tensor, defined by the relation

$$\delta x_\alpha = \sum_\beta u_{\alpha\beta} x_\beta \tag{C2}$$

between displacement $\delta\mathbf{x}$ and initial position $\mathbf{x}$ of any point in the body. Then the elastoresistance of any crystal is described mathematically by the fourth-rank tensor $\partial\sigma_{\mu\nu}/\partial u_{\alpha\beta}$, or more conveniently, for a cubic crystal, by the dimensionless tensor $-\sigma^{-1}\partial\sigma_{\mu\nu}/\partial u_{\alpha\beta}$, where σ is the scalar conductivity in the unstrained state ($\sigma_{\mu\nu} = \sigma\delta_{\mu\nu}$). The task of this appendix is to obtain this tensor hy calculating the strain variation of the current contrihutions (7), which in terms of components take the form

$$j_\mu^{(i)} = \frac{e^2}{kT} \sum_{\Delta\mathbf{p}^{(i)},s} f^{(0)} \tau(\Delta\epsilon^{(i)}) \sum_\nu v_\mu v_\nu E_\nu \tag{C3}$$

We shall base the calculation on assumptions (a) through (e) of Section 5. Assumptions (h) and (d), regarding existence of a $\tau(\Delta\epsilon)$ and nondegenerate statistics, are already contained in (C3). According to assumption (a), we shall neglect any effect of strain on the relations between $\mathbf{v}$, $\Delta\mathbf{P}$, and $\Delta\epsilon^{(i)} = |\epsilon - \epsilon^{(i)}|$. Thus we may replace $v_\mu v_\nu$ in (C3) by its average $L_{\mu\nu}^{(i)}$ over an energy shell, and treat this average for given $\Delta\epsilon^{(i)}$ as uninfluenced by strain:

$$v_\mu v_\nu \longrightarrow \tfrac{2}{3}\Delta\epsilon^{(i)} \begin{bmatrix} \frac{1}{m_1^*} & 0 & 0 \\ 0 & \frac{1}{m_2^*} & 0 \\ 0 & 0 & \frac{1}{m_3^*} \end{bmatrix} \equiv L_{\mu\nu}^{(i)} \tag{C4}$$

When the crystal is strained, the only things that we assume to change in (C3) are the population factor $f^{(0)}$ and the relaxation time $\tau(\Delta\epsilon^{(i)})$. For some groups of electrons — i.e., values of i and ϵ — the product $\tau f^{(0)}$ will be increased, and for others it will he decreased. If on the average this product is increased in the valleys whose conductivity tensors are most favorably oriented to the direction of $\mathbf{E}$, and decreased in the

others, the total current will be increased by the strain, and vice versa. When assumption (e) of Section 5 is fulfilled, so that two of the m^*'s, say m_1^* and m_2^*, are equal, the tensor (C4) takes the form

$$L_{\mu\nu}^{(i)} = \tfrac{2}{3}\Delta\epsilon^{(i)}\left[\frac{\delta_{\mu\nu}}{m_1^*} + \frac{K_\mu^{(i)}K_\nu^{(i)}}{K^{(i)2}}\left(\frac{1}{m_3^*} - \frac{1}{m_1^*}\right)\right] \tag{C5}$$

as is easily verified by inspection. Moreover, it is easily seen from symmetry that the only strain components which can alter $\epsilon^{(i)}$ in first order are the isotropic dilatation and the shear compounded out of an extension along $\mathbf{K}^{(i)}$ and a contraction in both directions at right angles. Mathematically expressed, we must have

$$\frac{\partial\epsilon^{(i)}}{\partial u_{\alpha\beta}} = \Xi_d\delta_{\alpha\beta} + \Xi_u K_\alpha^{(i)}K_\beta^{(i)}/K^{(i)} \tag{C6}$$

where Ξ_d and Ξ_u are constants independent of the valley i, the subscripts referring to "dilatational" and "uniaxial" effects respectively. The elastoresistance tensor is, for nondegenerate concentrations,

$$m_{\mu\nu\alpha\beta} \equiv -\frac{1}{\sigma}\frac{\partial\sigma_{\mu\nu}}{\partial u_{\alpha\beta}} = \frac{e^2}{kT\sigma}\sum_i\sum_{\Delta\mathbf{p}^{(i)},s} \left[\tau^{(i)}\frac{f^{(0)}}{kT}\frac{\partial\,|\,\epsilon^{(i)} - \epsilon_F\,|}{\partial u_{\alpha\beta}} - \sum_j f^{(0)}\frac{\partial\tau^{(i)}}{\partial\epsilon^{(j)}}\frac{\partial\epsilon^{(j)}}{\partial u_{\alpha\beta}}\right] L_{\mu\nu}^{(i)} \tag{C7}$$

where ϵ_F is the Fermi level, $\tau^{(i)}(\epsilon)$ is the relaxation time in the ith valley, and $L_{\mu\nu}^{(i)}$ is given by (C5). The second term in brackets in (C7) represents the effect of strain on the transition probability for inter-valley scattering.

We shall now combine and simplify the equations just given. The behavior of the Fermi level is simple: by assumption (a) of Section 4 it does not shift in shear, and for extrinsic concentrations it shifts with the band edge in compression. Mathematically,

$$\frac{\partial\epsilon_F}{\partial u_{\alpha\beta}} = \frac{1}{N_V}\sum_j\frac{\partial\epsilon^{(j)}}{\partial u_{\alpha\beta}} = \left(\Xi_d + \frac{\Xi_u}{3}\right)\delta_{\alpha\beta} \tag{C8}$$

where N_V is the number of valleys. By virtue of the fact that τ_i is a function only of $\Delta\epsilon$ and the differences $(\epsilon^{(i)} - \epsilon^{(j)})$,

$$\sum_j\frac{\partial\tau^{(i)}}{\partial\epsilon^{(j)}} = 0 \tag{C9}$$

and it is easily seen that when (C6) and (C8) are inserted into (C7) the Ξ_d terms disappear. Since by symmetry $\partial\tau^{(j)}/\partial\epsilon^{(i)} = \partial_\tau(i)/\partial\epsilon^{(j)}$, (C9)

implies

$$\sum_i \frac{\partial \tau^{(i)}}{\partial \epsilon^{(j)}} = 0 \tag{C10}$$

Using this and (C6) and (C8) in (C7), and processing further by (C5), we get

$$\begin{aligned} m_{\mu\nu\alpha\beta} &= \frac{e^2}{kT\sigma}\,\Xi_u \sum_i \sum_{\Delta \mathbf{P}^{(i)},s} \left[\pm \frac{\tau^{(i)}}{kT}\left(\frac{K_\alpha{}^{(i)}K_\beta{}^{(i)}}{K^{(i)2}} - \frac{\delta_{\alpha\beta}}{3}\right) \right. \\ &\qquad \left. - \sum_j \frac{\partial \tau^{(i)}}{\partial \epsilon^{(j)}}\,\frac{K_\alpha{}^{(j)}K_\beta{}^{(j)}}{K^{(j)2}} \right] f^{(0)} L_{\mu\nu}{}^{(i)} \\ &= \frac{2ne^2\Xi_u}{3kT\sigma}\left[\pm \frac{\langle \Delta\epsilon\tau\rangle}{kT}\left(\left\langle \frac{K_\mu{}^{(i)}K_\nu{}^{(i)}}{K^{(i)2}} \cdot \frac{K_\alpha{}^{(i)}K_\beta{}^{(i)}}{K^{(i)2}} \right\rangle_i - \frac{\delta_{\mu\nu}\delta_{\alpha\beta}}{9} \right) \right. \\ &\qquad \left. - N_V \left\langle \langle \Delta\epsilon \frac{\partial \tau^{(i)}}{\partial \epsilon^{(j)}} \rangle \cdot \frac{K_\mu{}^{(i)}K_\nu{}^{(i)}}{K^{(i)2}} \cdot \frac{K_\alpha{}^{(j)}K_\beta{}^{(j)}}{K^{(j)2}} \right\rangle_{i,j} \right] \left(\frac{1}{m_3{}^*} - \frac{1}{m_1{}^*} \right) \end{aligned} \tag{C11}$$

where the upper sign is for n-type, the lower for p, n is the total carrier concentration, angular brackets with a subscript i or i, j mean averages on valleys i or i and j, and angular brackets without subscripts mean Maxwellian averages as defined in Section 2. Substituting from (14) for the conductivity $\sigma = ne\mu$, we get finally

$$\begin{aligned} m_{\mu\nu\alpha\beta} &= 3\Xi_u \left[\pm \frac{1}{kT}\left(\left\langle \frac{K_\mu{}^{(i)}K_\nu{}^{(i)}}{K^{(i)2}} \cdot \frac{K_\alpha{}^{(i)}K_\beta{}^{(i)}}{K^{(i)2}} \right\rangle_i - \frac{\delta_{\mu\nu}\delta_{\alpha\beta}}{9} \right) \right. \\ &\qquad \left. - N_V \left\langle \frac{\langle \Delta\epsilon\, \partial\tau^{(i)}/\partial\epsilon^{(j)} \rangle}{\langle \Delta\epsilon\tau\rangle} \frac{K_\mu{}^{(i)}K_\nu{}^{(i)}}{K^{(i)2}} \cdot \frac{K_\alpha{}^{(j)}K_\beta{}^{(j)}}{K^{(j)2}} \right\rangle_{i,j} \right] \frac{(m_1{}^* - m_3{}^*)}{(m_1{}^* + 2m_3{}^*)} \end{aligned} \tag{C12}$$

As in (C7), the first term in square brackets in (C12) represents the effect of the strain on the relative populations of the different valleys, and the second term represents the effect on the inter-valley scattering probabilities. We may note the following features:

(1) The trace $\sum_\alpha m_{\mu\nu\alpha\alpha}$ vanishes identically, by virtue of (C9) etc. This means that an isotropic dilatation produces no elastoresistance under the assumptions we are using.

(2) The elastoresistance is proportional to the anisotropy of the effective mass within a valley.

(3) $m_{1212} = m_{44}$ vanishes for valleys of the (100) type, while $m_{1111} = m_{1122}$ ($m_{11} = m_{12}$) for valleys of the (111) type.

(4) The elastoresistance is proportional to $1/T$ at temperatures low enough for inter-valley scattering to be frozen out. Moreover, when $kT \gg$ the inter-valley $\hbar\omega(ij)$ of Section 3, the variation of $\partial\tau_i/\partial\epsilon_j$ with energy

$\Delta\epsilon$ relative to the band edge is easily shown to be one of proportionality to $\tau/\Delta\epsilon$, if impurity scattering is negligible. Under these conditions (probably never achieved by Si and Ge in the extrinsic range) the elastoresistance is again proportional to $1/T$, but with a larger factor of proportionality than at low T.

NOTATIONS

A	dimensionless average involving relaxation time, Equation (68)
B	dimensionless function of mass anisotropy, Equation (39)
$C(\mathbf{K}, \mathbf{K}')$	factor in matrix element for a scattering process $\mathbf{K} \rightarrow \mathbf{K}'$, Equation (A6)
c	velocity of light; magnetoresistance constant, Equation (74)
D_{ij}	factor in matrix element for scattering from valley i to valley j, Equation (16)
$\mathbf{E}$	electric field
e	electronic charge
$F_{\mu\nu\alpha\beta}$	factor determining the anisotropy of the magnetoconductance tensor Equations (70), (71)
$F_{\mu\nu\alpha\beta}^{(i)}$	contribution of the ith valley to above, Equation (69)
f	distribution function for charge carriers.
$f^{(0)}$	same in absence of perturbing fields, Equation (1)
$\mathbf{f}^{(1)}$ etc.	change of f in perturbing fields, Equations (4), (31), (60)
G	dimensionless average involving relaxation time, Equation (57)
$\mathbf{H}$	magnetic field
$\hbar$	Planck's constant/2π
$\mathbf{j}$	density of electric current
$\mathbf{K}$	wave number vector for a charge carrier
$\mathbf{K}^{(i)}$	value of $\mathbf{K}$ for the ith band edge point (center of the ith valley)
k	Boltzmann's constant
$L_{\mu\nu}^{(i)}$	average of $v_\mu v_\nu$ over an energy shell in the ith valley

$M(\mathbf{K}, \mathbf{K}')$, M_{ij}	matrix element for lattice scattering, Equation (A6) or (16)
m	normal electron mass
$m_\lambda{}^*$	effective mass in λth principal direction of a valley
$m^{(I)}$	inertial average of the $m_\lambda{}^*$, defined by Equation (15)
$m_{\mu\nu\alpha\beta}$	elastoresistance tensor $-\sigma^{-1}\partial\sigma_{\mu\nu}/\partial u_{\alpha\beta}$
N, N_α	number of quanta (phonons) in a given lattice mode
N_V	number of valleys or band edge points
n	number of free charge carriers per unit volume
$\mathbf{P}$	crystal momentum $\hbar\mathbf{K}$
Q_e	electronic part of thermoelectric power
$\mathbf{q}$	wave number vector for a lattice mode
R	Hall constant
$S(\mathbf{K}, \mathbf{K}')$	transition probability $\mathbf{K}$ to unit $d\mathbf{K}'$ at $\mathbf{K}'$, Equation (A1)
s	spin quantum number of a charge carrier
T	absolute temperature
t	time
$u_{\alpha\beta}$, u_r	strain tensor components
$\mathbf{v}$	group velocity of a charge carrier
$W_a(ij, \alpha)$	transition probability from valley i to valley j with absorption of a phonon of branch α
$W_e(ij, \alpha)$	same but with emission
w_1 , w_2	constants of dimension (time)$^{-1}$, measuring coupling of carriers to intra- and intervalley modes, respectively, Equations (21)–(23)
x, y, z	rectangular coordinates
α (when not subscript)	index labeling branches of vibrational spectrum
Υ	differential operator describing rotation of distribution by magnetic field, Equation (62)
$\Delta\epsilon$	energy of a carrier relative to the band edge ($\Delta\epsilon \geqq 0$)
$\Delta\mathbf{P}$, $\Delta\mathbf{K}$	departure of crystal momentum or wave vector from valley center
$\delta_{\mu\nu}$	Kronecker delta

$\delta_{\mu\nu\sigma}$	antisymmetric coefficient = ± 1 or 0, Equation (33)
$\delta\epsilon$, $\delta\mathbf{v}$, etc.	changes induced by strain
ϵ	energy of an electron
ϵ_b	band edge energy
$\epsilon^{(i)}$	energy of the center of the ith valley (normally = ϵ_b)
Θ	Debye temperature
κ	dielectric constant
μ	drift mobility
μ_H	Hall mobility
Ξ_d , Ξ_u	deformation potentials, Equation (C6)
ξ	transformed coordinate, equation (A15)
ρ	resistivity
σ	conductivity
σ_0	conductivity in the absence of magnetic fields or other perturbations
$\sigma_{\mu\nu\alpha}$, $\sigma_{\mu\nu\alpha\beta}$	coefficients in the expansion of conductivity in powers of H, Equation (65)
$\sigma_{\mu\nu\alpha\beta}^{(i)}$	contribution of ith valley to magnetoconductivity
τ	relaxation time of charge carriers
$\tau^{(i)}$	ditto for carriers in valley i
φ	transformed wave vector, Equation (B1)
ω	angular frequency of a lattice mode or an rf field